10816329.trn

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NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS	4	DEC 18	CA/CAplus patent kind codes updated
NEWS	5	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS	6	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS	7	DEC 27	CA/CAplus enhanced with more pre-1907 records
NEWS	8	JAN 08	CHEMLIST enhanced with New Zealand Inventory of Chemicals
NEWS	9	JAN 16	CA/CAplus Company Name Thesaurus enhanced and reloaded
NEWS	10	JAN 16	IPC version 2007.01 thesaurus available on STN
NEWS	11	JAN 16	WPIDS/WPINDEX/WPIX enhanced with IPC 8 reclassification data
NEWS	12	JAN 22	CA/CAplus updated with revised CAS roles
NEWS	13	JAN 22	CA/CAplus enhanced with patent applications from India
NEWS	14	JAN 29	PHAR reloaded with new search and display fields
NEWS	15	JAN 29	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS	16	FEB 15	PATDPASPC enhanced with Drug Approval numbers
NEWS	17	FEB 15	RUSSIAPAT enhanced with pre-1994 records
NEWS	18	FEB 23	KOREAPAT enhanced with IPC 8 features and functionality
NEWS	19	FEB 26	MEDLINE reloaded with enhancements
NEWS	20	FEB 26	EMBASE enhanced with Clinical Trial Number field
NEWS	21	FEB 26	TOXCENTER enhanced with reloaded MEDLINE
NEWS	22	FEB 26	IFICDB/IFIPAT/IFIUDB reloaded with enhancements
NEWS	23	FEB 26	CAS Registry Number crossover limit increased from 10,000 to 300,000 in multiple databases
NEWS	24	MAR 15	WPIDS/WPIX enhanced with new FRAGHITSTR display format
NEWS	25	MAR 16	CASREACT coverage extended
NEWS	26	MAR 20	MARPAT now updated daily
NEWS	27	MAR 22	LWPI reloaded

NEWS EXPRESS NOVEMBER 10 CURRENT WINDOWS VERSION IS V8.01c, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 25 SEPTEMBER 2006.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8
NEWS X25	X.25 communication option no longer available

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FILE 'HOME' ENTERED AT 16:33:18 ON 22 MAR 2007

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 16:33:25 ON 22 MAR 2007
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STRUCTURE FILE UPDATES: 21 MAR 2007 HIGHEST RN 927866-99-7
DICTIONARY FILE UPDATES: 21 MAR 2007 HIGHEST RN 927866-99-7

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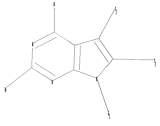
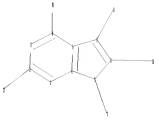
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>
Uploading C:\Program Files\Stnexp\Queries\10816329.str





chain nodes :
12 13 15 16
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
2-12 4-10 7-15 8-16 9-13
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
2-12 4-10 6-9 7-15 8-9 8-16 9-13
exact bonds :
5-7 7-8
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

G1:C,H,Cy

G2:H,Cl,Br,F,I,Cy,Ak

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
12:Atom 13:CLASS 15:CLASS 16:CLASS

L1 STRUCTURE UPLOADED

=> s l1 sam
SAMPLE SEARCH INITIATED 16:33:41 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 792 TO ITERATE

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100.0% PROCESSED      792 ITERATIONS                              15 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        14152 TO    17528
PROJECTED ANSWERS:              68 TO      532

L2           15 SEA SSS SAM L1

=> d l1
L1 HAS NO ANSWERS
L1                STR
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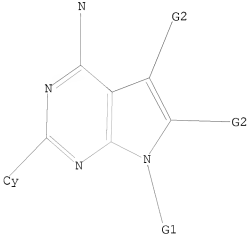


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G1 C,H,Cy
G2 H,Cl,Br,F,I,Cy,Ak


Structure attributes must be viewed using STN Express query preparation.


=> s l1 full
FULL SEARCH INITIATED 16:33:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    16439 TO ITERATE

100.0% PROCESSED    16439 ITERATIONS                            284 ANSWERS
SEARCH TIME: 00.00.01

L3          284 SEA SSS FUL L1

=> fil capl
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              172.10     172.31

FILE 'CAPLUS' ENTERED AT 16:33:58 ON 22 MAR 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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FILE COVERS 1907 - 22 Mar 2007 VOL 146 ISS 13
FILE LAST UPDATED: 21 Mar 2007 (20070321/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3
L4 31 L3

=> s l4 not (2007/so or 2006/so or 2005/so)
151426 2007/SO
811675 2006/SO
872221 2005/SO
L5 31 L4 NOT (2007/SO OR 2006/SO OR 2005/SO)

=> s l5 ibib hitstr abs 1-31
MISSING OPERATOR L5 IBIB
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.

=> d l5 ibib hitstr abs 1-31

L5 ANSWER 1 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:139424 CAPLUS
DOCUMENT NUMBER: 146:258999
TITLE: Composition comprising a benzodiazepine agonist and a benzodiazepine antagonist
INVENTOR(S): Malnville, Pierre
PATENT ASSIGNEE(S): Can.
SOURCE: U.S. Pat. Appl. Publ., 5pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20070047672	A1	20070222	US 2005-208506	20050822
CA 2556163	A1	20070222	CA 2006-2556163	20060815
PRIORITY APPLN. INFO.:			US 2005-208506 A	20050822

IT 157013-32-6, U 89843A
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(composition comprising a benzodiazepine agonist and a benzodiazepine antagonist)
RN 157013-32-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

AB This invention relates to a composition comprising a benzodiazepine agonist, a benzodiazepine antagonist, and a pharmaceutical acceptable carrier in an effective ratio so as to preserve the therapeutic effects of the benzodiazepine agonist while modulating the side effects of the benzodiazepine agonist. For example, 44 yr old female suffering from a chronic reflex sympathetic dystrophy type 1 of her right knee with severe anxiety was treated simultaneously with 5 mg of midazolam i.v. and 500 mg of flunarazyl i.v.. At this point, she rated her pain at 5/10. Less than 15 min after treatment, her pain went down to 0/10 without any sedative effects.

L5 ANSWER 2 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L5 ANSWER 2 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:952415 CAPLUS
DOCUMENT NUMBER: 145:342443
TITLE: Compositions comprising NEP inhibitors, endogenous endothelin inhibitors and diuretics for treatment of cardiovascular disease
INVENTOR(S): Straub, Matthias; Witte, Klaus; Ziegler, Dieter; Fischer, Yvan
PATENT ASSIGNEE(S): Solvay Pharmaceuticals GmbH, Germany
SOURCE: U.S. Pat. Appl. Publ., 15pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20060209914	A1	20060914	US 2006-356080	20060217
PRIORITY APPLN. INFO.:			US 2005-653954P	P 20050218

OTHER SOURCE(S): MARPAT 145:342443
IT 342632-54-2
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compns. comprising NEP inhibitors, endogenous endothelin inhibitors and diuretics for treatment of cardiovascular disease)
RN 342632-54-2 CAPLUS
CN 2-Pyrrolidinecarboxamide, 4-hydroxy-1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

AB A novel combination therapy for cardiovascular diseases or conditions, including administering a synergistic combination of at least one inhibitor of neutral endopeptidases, at least one inhibitor of the endogenous endothelin producing system and at least one diuretic, preferably a thiazide diuretic or an adenosine A1 antagonist. For example, capsule was formulated containing daglutril calcium 252 mg and hydrochlorothiazide 50 mg.

L5 ANSWER 3 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:847629 CAPLUS
DOCUMENT NUMBER: 145:278270
TITLE: Pharmaceutical compositions comprising inhibitors of neutral endopeptidase and inhibitors of the endogenous endothelin and diuretics for the treatment of cardiovascular diseases
INVENTOR(S): Witte, Klaus; Ziegler, Dieter; Straub, Matthias; Fischer, Yvan
PATENT ASSIGNEE(S): Solvay Pharmaceuticals GmbH, Germany
SOURCE: PCT Int. Appl., 39pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006087371	A1	20060824	WO 2006-EP60057	20060217
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, ZW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
EP 2005-101235	A	20050218
PRIORITY APPLN. INFO.:		

OTHER SOURCE(S): MARPAT 145:278270
IT 342632-54-2D, derivs.
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmaceutical compns. comprising inhibitors of neutral endopeptidase and inhibitors of the endogenous endothelin and diuretics for the treatment of cardiovascular diseases)
RN 342632-54-2 CAPLUS
CN 2-Pyrrolidinecarboxamide, 4-hydroxy-1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 3 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB A novel combination therapy is described for cardiovascular diseases or conditions, by administering a synergistic combination of at least one inhibitor of neutral endopeptidase, at least one inhibitor of the endogenous endothelin producing system and at least one diuretic, preferably a thiazide diuretic or an aldosterone AI antagonist. For example, capsules contained daglutril calcium, and hydrochlorothiazide, corn starch, lactose and ST sodate.

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:31629 CAPLUS

DOCUMENT NUMBER: 142:392424

TITLE: Preparation of aminopyrrolopyrimidines as adenosine A1 receptor antagonists.

INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.

PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA

SOURCE: U.S., 46 pp., Cont.-in-part of Appl. No PCT/US99/11335.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6878716	B1	20050412	US 1999-454674	19991202
WO 9961135	A1	19991209	WO 1999-US12135	19990601

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW

RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2393179	A1	20010607	CA 2000-2393179	20001201
WO 2001037777	A1	20010607	WO 2000-US33702	20001201

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

EP 1246623	A1	20021009	EP 2000-980911	20001201
EP 1246623	B1	20060809		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR

JP 2003519102	T	20030617	JP 2001-541589	20001201
AU 784678	B2	20060713	AU 2001-24279	20001201
AT 335489	T	20060915	AT 2000-980911	20001201
ES 1731529	A1	20061213	ES 2006-16543	20001201

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ZA 2002004153	A	20040715	ZA 2002-4153	20020524

PRIORITY APPLN. INFO.: US 1998-87902P P 19980602

US 1999-123216P P 19990308

L5 ANSWER 4 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

US 1999-124527P P 19990326

WO 1999-US12135 A2 19990601

US 1999-454074 A 19991202

US 1999-454075 A 19991202

US 1999-454254 A 19991202

EP 2000-980911 A3 20001201

WO 2000-US33702 W 20001201

OTHER SOURCE(S): MARPAT 142:392424

IT 251946-53-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aminopyrrolopyrimidines as adenosine A1 receptor antagonists)

RN 251946-53-9 CAPLUS

CN Acetamide, N-[1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-4-piperidinyl]- (9CI) (CA INDEX NAME)

IT 347631-98-1

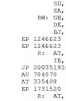
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of aminopyrrolopyrimidines as adenosine A1 receptor antagonists)

RN 347631-98-1 CAPLUS

CN Acetamide, N-[1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-3-piperidinyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 4 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



GI

AB Title compds. [I; R1 = trans-4-hydroxycyclohexyl, 2-methylaminoacetoxylaminocyclohexyl, acetylaminoethyl, methylaminoacetoxylaminoethyl; R3 = (substituted) Ph, pyrrolyl, thienyl, furyl, thiazolyl, imidazolyl, pyrazolyl, pyrazinyl, purinyl, quinazolinyl, etc.; R5 = H, (substituted) alkyl, amino, Ph, pyrrolyl, furyl, thienyl, imidazolyl, benzoxazolyl, benzothiazolyl, triazolyl, tetrazolyl, pyrazolyl, pyridinyl, pyrazinyl, pyridazinyl, pyrimidinyl, naphthyl, quinolyl, indolyl, etc.; R6 = H, (substituted) alkyl, cycloalkyl), were prepared Thus, 4-chloro-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine and trans-4-hydroxycyclohexylamine were heated in MeIBO at 130° for 5 h to give 75% 4-(4-trans-hydroxycyclohexylamino-6-methyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine. I showed A1 receptor binding with Ki = 2.2-15000 nM.

REFERENCE COUNT: 120 THERE ARE 120 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:88297 CAPLUS
DOCUMENT NUMBER: 140:146159
TITLE: Preparation and use of substituted pyrrolo[2,3-d]pyrimidines as selective adenosine A3 receptor antagonists
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David
PATENT ASSIGNEE(S): GPC Pharmaceuticals, Inc., USA
SOURCE: U.S., 75 pp., Cont.-in-part of Appl. No. PCT/US99/21135.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6696706	B1	20040203	US 1999-454075	19991202
WO 9962518	A1	19991209	WO 1999-US21135	19990601
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RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
CA 2393379	A1	20010607	CA 2000-2393179	20001201
WO 2001089577	A2	20011127	WO 2000-US32702	20001201
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EP 1246623	A1	20021009	EP 2000-988011	20001201
EP 1246623	B1	20060909		
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JP 2003519102	T	20030617	JP 2001-541509	20001201
AU 784878	B2	20060713	AU 2001-24470	20001201
AT 335489	T	20060915	AT 2000-988011	20001201
ES 2271520	A1	20061213	ES 2006-16543	20001201
PRIORITY APPLN. INFO.:			US 1998-87702P	P 19980602
			US 1999-123216P	P 19990308

L5 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

		US 1999-454075	P 19991202
		WO 1999-US21135	A2 19990601
		US 1999-454074	A 19991202
		US 1999-454075	A 19991202
		US 1999-454254	A 19991202
		EP 2000-988011	A3 20001201
		WO 2000-US32702	W 20001201

OTHER SOURCE(S): MARPAT 140:146159
IT 343673-98-1P 343632-74-8P 343632-42-8P 343632-47-3P 343632-48-4P 343632-49-5P 343632-64-6P 343632-74-4P 343632-75-7P 343632-84-8P 343632-85-9P 343632-86-0P 343632-87-1P 343632-88-2P 343632-99-3P 343632-90-6P 343969-90-2P 653600-35-2P 653600-36-3P
RL: PAC (Pharmacological activity); SYN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as selective adenosine A3 receptor antagonists)
RN 343673-98-1 CAPLUS
CN Acetamide, N-[1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-3-piperidinyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343632-42-8 CAPLUS
CN 3-Azetidinemethanol, 1-[2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

RN 343632-47-3 CAPLUS
CN 3-Pyridinecarboxylic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN 343632-48-4 CAPLUS
CN 3-Pyridinecarboxamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

L5 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343632-49-5 CAPLUS
CN 3-Pyridinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

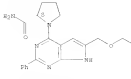
RN 343632-65-5 CAPLUS
CN Acetic acid, [[6-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]methoxy]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-66-6 CAPLUS
CN Acetic acid, [[6-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]methoxy]- (9CI) (CA INDEX NAME)

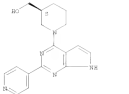
Absolute stereochemistry.

L5 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 343632-74-6 CAPLUS
CN 3-Piperidineethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3S)- (9CI) (CA INDEX NAME)

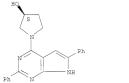
Absolute stereochemistry.



RN 343632-75-7 CAPLUS
CN 3-Piperidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3R)- (9CI) (CA INDEX NAME)

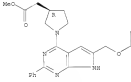
Absolute stereochemistry.

L5 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



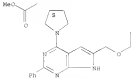
RN 343632-86-0 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



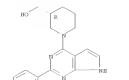
RN 343632-87-1 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



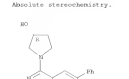
RN 343632-88-2 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3R)- (9CI) (CA INDEX NAME)

L5 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 343632-94-8 CAPLUS
CN 3-Pyrrolidinol, 1-(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

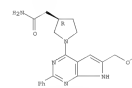


RN 343632-85-9 CAPLUS
CN 3-Pyrrolidinol, 1-(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

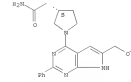
L5 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry.



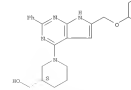
RN 343632-89-3 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-90-6 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3S)- (9CI) (CA INDEX NAME)

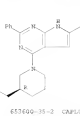
Absolute stereochemistry.



RN 343969-98-2 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-

L5 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
pyrrolo[2,3-d]pyrimidin-4-yl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 657609-35-2 CAPLUS
CN Acetamide, N-[(3S)-1-[5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

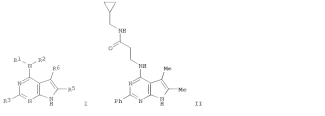
RN 633609-36-3 CAPLUS
CN Acetamide, N-[(3S)-1-[5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-3-piperidinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
A3 adenosine receptors in a subject.
REFERENCE COUNT: 128 THERE ARE 128 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

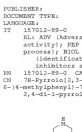
L5 ANSWER 5 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

GI



AB The title compds. [I; R1 = H and R2 = cyclopropylmethylaminocarbonylethyl, cis-3-hydroxycyclopentyl, acetamidobutyl, etc.; or NR1R2 = 3-acetamidopiperazino, 3-hydroxypyrrolidino, 3-methoxycarbonylmethylpyrrolidino, etc.; R3 = (un)substituted cycloalkyl, aryl; R5 = H, alkyl, aryl; R6 = H, alkyl, cycloalkyl] which specifically inhibit the adenosine A3 receptor and are useful for treating a disease associated with A3 adenosine receptor, were prepared. Thus, 4-chloro-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine was reacted with 4-trans-hydroxycyclohexylamine in DMSO at 170°C for 5 h to yield I [R1 = H; R2 = trans-4-hydroxycyclohexyl; R3 = Ph; R5, R6 = Me] in 75% yield after purification which showed Ki of 13.9 nM against adenosine receptor A1 binding. Some of the compds. I such as II exhibited at least 10 times more selective binding to adenosine receptor A3 than other receptor subtype. Claimed use of I includes administration of a systemic formulation (i.e. ophthalmic) for the treatment of a disease associated with

L5 ANSWER 6 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:726750 CAPLUS
DOCUMENT NUMBER: 139:333072
TITLE: Identification and prediction of promiscuous aggregating inhibitors among known drugs
AUTHOR(S): Seidler, Jamey McGovern; Susan L.; Doman, Thompson N.; Shoichet, Brian K.
CORPORATE SOURCE: Department of Molecular Pharmacology and Biological Chemistry, Northwestern University, Chicago, IL, 60611, USA
SOURCE: Journal of Medicinal Chemistry (2003), 46(21), 4477-4486
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 157012-89-0
RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); PEP (Physical, engineering or chemical process); PYP (Physical process); BIOL (Biological study); PROC (Process)
(identification and prediction of promiscuous aggregating enzyme inhibitors among known drugs)
RN 157012-89-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-methylphenyl)-7-[2-[1-piperazinyl]ethyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



AB Some small mols., often hits from screening, form aggregates in solution that inhibit many enzymes. In contrast, drugs are thought to act specifically. To investigate this assumption, 50 unrelated drugs were tested for promiscuous inhibition via aggregation. Each drug was tested against three unrelated model enzymes: β-lactamase, chymotrypsin, and malate dehydrogenase, none of which are considered targets of these drugs. To be judged promiscuous, the drugs had to inhibit all three enzymes, do so in a

L5 ANSWER 6 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
time-dependent manner, be sensitive to detergent and to enzyme concn., and
form particles detectable by light scattering. Of the 50 drugs tested, 43
were nonpromiscuous by these criteria. Surprisingly, four of the drugs showed promiscuous, aggregation-based inhibition at concns. below 100 μM: clotrimazole, benzyl benzoate, nicardipine, and delavirdine. Three other drugs also behaved as aggregation-based inhibitors, but only at high
concns. (about 650 μM). To investigate possible structure-activity relationships among promiscuous drugs, five analogs of the antifungal clotrimazole were studied. Three of these, miconazole, econazole, and ruliconazole, were promiscuous but the other two, fluconazole and ketoconazole, were not. Using recursive partitioning, these suggestive results were used to develop a model for predicting aggregate-based promiscuity. This model correctly classified 548 of 111 compds.--- 47 aggregators and 64 nonaggregators-- that have been studied for this effect. To evaluate the model, it was used to predict the behaviour of 75 drugs not previously investigated for aggregation. Several preliminary points emerge. Most drugs are not promiscuous, even at high concns. Nevertheless, at high enough concns. (20-400 μM), some drugs can aggregate and act promiscuously, suggesting that aggregation may be common
among small mols. at micromolar concns., at least in biochem. buffers.
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 7 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:570644 CAPLUS
DOCUMENT NUMBER: 139:133575
TITLE: Preparation of bicyclic pyrimidinyl derivatives as adenosine receptor ligands
INVENTOR(S): Castelhano, Arlindo L.; McFadden, Bryan
PATENT ASSIGNEE(S): OSI Pharmaceuticals Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 105 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

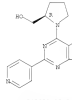
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20013739427	A1	20030724	US 2002-227770	20020823
PRIORITY APPLN. INFO.:			US 2002-227770	20020823

OTHER SOURCE(S): MARPAT 139:133575
IT 343631-98-1P 343632-22-4P 343632-23-5P 343632-24-6P 343632-25-7P 343632-26-8P 343632-28-0P 343632-29-1P 343632-34-8P 343632-42-8P 343632-47-3P 343632-48-4P 343632-49-5P 565234-94-5P
RL: PAC (Pharmacological activity); PEN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bicyclic pyrazolo- imidazo- and triazolopyrimidinyl derivs. as adenosine receptor ligands)
RN 343631-98-1 CAPLUS
CN Acetamide, N-[1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-3-piperidinyl]- (9CI) (CA INDEX NAME)

RN 343632-22-4 CAPLUS
CN 2-Pyrrolidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAME)

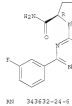
Absolute stereochemistry.

L5 ANSWER 7 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



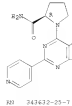
RN 343632-23-5 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-24-6 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl-, (2R)- (9CI) (CA INDEX NAME)

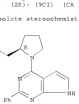
Absolute stereochemistry.



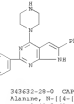
RN 343632-25-7 CAPLUS

L5 ANSWER 7 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Pyrrolidinemethanol, 1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

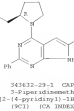


RN 343632-26-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 4-phenyl-4-(1-piperazinyl)-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)



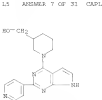
RN 343632-28-0 CAPLUS
CN Alanine, N-[[4-[(2R)-2-(hydroxymethyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-6-yl]methyl]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

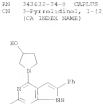


RN 343632-29-1 CAPLUS
CN 3-Piperidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

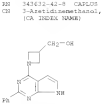
L5 ANSWER 7 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 343632-34-8 CAPLUS
CN 3-Pyrrolidino1, 1-(5,6-d)phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)- (9CI) (CA INDEX NAME)



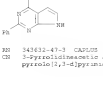
RN 343632-42-8 CAPLUS
CN 3-Azetidinemethanol, 1-[2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)- (9CI) (CA INDEX NAME)



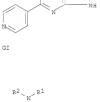
RN 343632-49-3 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester (9CI) (CA INDEX NAME)

L5 ANSWER 7 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
d]pyrimidin-4-yl]-, (2R,4R)-rel- (9CI) (CA INDEX NAME)

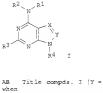
Relative stereochemistry.



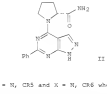
GI



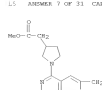
AB Title compds. I [Y = N, CR5 and X = N, CR6 wherein X, Y are both N or when Y = CR5, X = N or when X = CR6, Y = N; R1-2 = H, alkoxy, aminoalkyl, etc; R3-4 = H, alkyl, aryl, alkylaryl] are prepared For instance, 3-amino-4-carbamoylpyrazole is acylated with benzoyl chloride (Pyridine, 80°, 5-6 h), cyclized to the corresponding pyrazolopyrimidine (water, KCCO3, 100°, 16 h), converted to the chloride (POCl3, 106°, 2 h) and used for reactions with various amines to give the example compds., e.g., II. II has Ki = 76.7 nM for the adenosine A1 receptor, Ki = 242.7 nM for A2a and Ki = 1480.5 nM for A2b. I are useful for the treatment of.



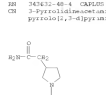
I



II



RN 343632-48-4 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)



RN 343632-49-5 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

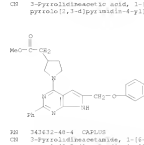
RN 565234-94-8 CAPLUS
CN 2-Pyrrolidinemethanol, 4-hydroxy-1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-

L5 ANSWER 8 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2007:151094 CAPLUS
DOCUMENT NUMBER: 139:85365
TITLE: Preparation of pyrrolopyrimidine A2b selective antagonist compounds, method of synthesis and therapeutic use
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Steinig, Arno
PATENT ASSIGNEE(S): Gi Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 223 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

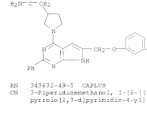
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005053361	A2	20050707	WO 2004-US40890	20021220
WO 2005053361	A3	20051224		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW: GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2470044	A1	20050707	CA 2002-2470044	20021220
AU 2002366801	A1	20050707	AU 2002-366801	20021220
US 2005236007	A1	20051221	US 2002-316005	20021220
EP 1467995	A2	20041020	EP 2002-805644	20021220
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
BR 2002015179	A	20040615	BR 2002-15179	20021220
JP 2005525305	A	20050825	JP 2003-554221	20021220
CN 1816551	A	20060809	CN 2002-828272	20021220
PRIORITY APPLN. INFO.:			US 2001-343443P	P 20011220
			WO 2002-US40890	W 20021220

OTHER SOURCE(S): CASREACT 139:85365; MARPAT 139:85365
IT 343632-47-7P, 1-[6-[(3-Chlorophenoxy)methyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]pyrrolidin-3-yl]acetic acid methyl ester 343632-48-4P, 2-(1-[6-[(3-Chlorophenoxy)methyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]pyrrolidin-3-yl)acetamide 343632-49-5P, 1-[6-[(3-Chlorophenoxy)methyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]piperidin-3-yl]methanol 553631-86-0P, 2-[1-[6-[(3-Chlorophenoxy)methyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]pyrrolidin-2-yl]ethanol 553631-95-1P, [1-[6-[(3-Chlorophenoxy)methyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]pyrrolidin-3-yl]acetic acid 553632-01-2P, [1-[6-[(3-Chlorophenoxy)methyl]-2-phenyl-7H-pyrrolo[2,7-d]pyrimidin-4-yl]azetidin-3-yl]methanol 553632-30-7P, 1-[4-[6-[(3-Chlorophenoxy)methyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]piperazin-1-yl]ethanone 553632-31-8P

L5 ANSWER 8 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
, 1-[6-[3-Chlorophenoxymethyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]azetidin-3-ol
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preps. of pyrrolopyrimidine A2b selective antagonist compds., method of synthesis and therapeutic use)
RN 347672-45-3 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester (9CI) (CA INDEX NAME)

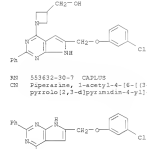


RN 347672-48-4 CAPLUS
CN 3-Pyrrolidinecarboxamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

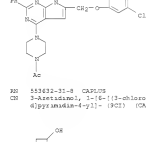


RN 347672-49-5 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

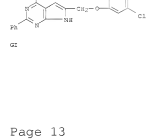
L5 ANSWER 8 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 553632-30-7 CAPLUS
CN Piperazine, 1-acetyl-4-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

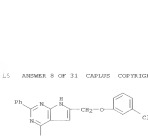


RN 553632-31-8 CAPLUS
CN 3-Azetidinol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

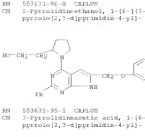


GI

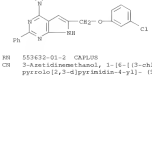
L5 ANSWER 8 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 553631-86-9 CAPLUS
CN 2-Pyrrolidinethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

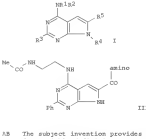


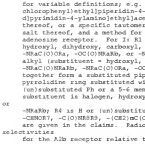
RN 553631-95-1 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)



RN 553632-01-2 CAPLUS
CN 3-Azetidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

L5 ANSWER 8 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)





AB The subject invention provides pyrrolopyrimidines (shown as I; see below for variable definitions; e.g. N-[2-[6-[1-[2-[2-chlorophenyl]ethyl]piperidin-4-yloxymethyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-ylamino]ethyl]acetamide (II)) or a specific enantiomer thereof, or a specific tautomer thereof, or a pharmaceutically acceptable salt thereof, and a method for treating a disease associated with the A2b adenosine receptor. For I: R1 is a (un)substituted alkyl (substituent = hydroxyl, dihydroxy, carboxyl, -C(O)NHaRb, -SHaRb, -SHaC(O)HaRb, -NHaC(O)Ha, -OC(O)NHaRb, or -NHC(O)Ra). R2 is H or a (un)substituted alkyl (substituent = hydroxyl, dihydroxyl, carboxyl, -C(O)NHaRb, -NHaC(O)NHaRb, -NHaC(O)Ra, -OC(O)NHaRb, or -NHC(O)Ra); or R1, R2 and N together form a substituted piperazine, substituted azetidine, or a pyrrolidine ring substituted with -(CR2)2OH or -CHR2C(O)OH. R3 is a (un)substituted Ph or a 5-6 membered heteroaryl ring, wherein the substituent is halogen, hydroxyl, cyano, (C1-C15)alkyl, (C1-C15)alkoxyl or -NHaRb; R4 is H or (un)substituted (C1-C15)alkyl; R5 is -(CR2)mOR6, -CHNOR7, -C(O)NHSR8, -(CR2)mC(O)OR10, -(CR2)kC(O)NR11R12; addn. details are given in the claims. Radioligand binding assays yielded selectivities for the A2b receptor relative to the A1, A2a and A3 receptors for 9 examples of I, e.g. 26 times for II. About 26 example preps. of I and intermediates and characterization data for hundreds of I and intermediates are included. For example, III can be prepared by reacting 6-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine with PhSO2Cl and a reducing agent in the presence of solvent to produce 7-benzenesulfonyl-4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine, which was reacted with CO2 in the presence of LDA and a solvent to produce lithium 7-benzenesulfonyl-4-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine-6-carboxylate, which was reacted with AcNHCH2CH2NH2 in the presence of solvent to give 6-(2-acetylaminoethylamino)-7-benzenesulfonyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, which was deprotected with a hydroxide base and subsequently condensed with amines.

L5 ANSWER 9 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:454286 CAPLUS
DOCUMENT NUMBER: 139:36534
TITLE: Preparation of arylpyrrolopyrimidines as adenosine A1 and A3 receptor inhibitors
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Werner, Douglas S.; Mutter, David
PATENT ASSIGNEE(S): GSI Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 170 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003048132	A2	20030612	WO 2002-US38055	20021127
WO 2003048132	A3	20030904		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
CA 2468673	A1	20030612	CA 2002-2468673	20021127
AU 2002360476	A1	20030617	AU 2002-360476	20021127
EP 1459811	A2	20040901	EP 2002-795691	20021127
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
US 20050090517	A1	20050428	US 2005-497451	20021127
JP 2005529062	T	20050929	JP 2003-549312	20021127
PRIORITY APPLN. INFO.:			US 2001-3352739 P	20011130
			US 2001-3372749 P	20011130
			WO 2002-US38055 W	20021127

OTHER SOURCE(S): MARPAT 139:36534
IT 541503-99-7P 541503-93-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of arylpyrrolopyrimidines as adenosine A1 and A3 receptor inhibitors)
RN 541503-99-7 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 4-(3,3a,4,6,7,7a-hexahydro-5H-imidazo[4,5-c]pyridin-5-yl)-2-phenyl- (9CI) (CA INDEX NAME)

L5 ANSWER 9 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343632-42-8 CAPLUS
CN 3-Azidobenzenethanol, 1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)- (9CI) (CA INDEX NAME)

RN 343632-47-3 CAPLUS
CN 3-Pyridineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester (9CI) (CA INDEX NAME)

RN 343632-48-4 CAPLUS
CN 3-Pyridinecarboxamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

L5 ANSWER 9 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 541503-93-9 CAPLUS
CN 2-Pyrrolidinecarboxamide, 4-hydroxy-1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 343632-34-8P 343632-42-8P 343632-47-3P
343632-48-4P 343632-49-5P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of arylpyrrolopyrimidines as adenosine A1 and A3 receptor inhibitors)
RN 343632-34-8 CAPLUS
CN 3-Pyrrolidinol, 1-(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)- (9CI) (CA INDEX NAME)

RN 343632-49-5 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

GI

AB Arylpyrrolopyrimidines I [m = 0-3; R = halogen, alkyl, alkoxy, OH, NH2, alkylamino; R1 = H, (un)substituted alkyl, aryl, aralkyl; R2 = (un)substituted imidazole, pyrazole, attached through C] which specifically inhibit the adenosine A1 and A3 receptors were prepared Thus, 6-chloro-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine was treated with histamine to give the 4-[2-[1H-imidazol-2-yl]ethylamino analog which had A3 inhibiting activity ≥10 times greater than that of reference compds:

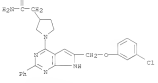
L5 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:302617 CAPLUS
DOCUMENT NUMBER: 138:321287
TITLE: Preparation of deazapurines as adenosine A3 receptor antagonists.
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
PATENT ASSIGNEE(S): OSI Pharmaceuticals, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 77 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20030073708	A1	20030417	US 2001-4405	20011130
US 6673802	B2	20040106		
PRIORITY APPLN. INFO.:			US 2000-250748P	P 20001201

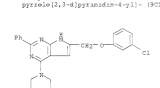
OTHER SOURCE(S): MARPAT 138:321287
IT 343631-98-3P 343632-34-8P 343632-42-8P
343632-47-3P 343632-48-4P 343632-49-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of deazapurines as adenosine A3 receptor antagonists)
RN 343631-98-3 CAPLUS
CN Acetamide, N-[1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-3-piperidinyl]- (9CI) (CA INDEX NAME)

RN 343632-34-8 CAPLUS
CN 3-Pyrrolidinol, 1-[2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

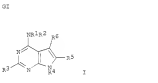
L5 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 343632-42-8 CAPLUS
CN 3-Azetidinemethanol, 1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)- (9CI) (CA INDEX NAME)

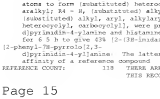


RN 343632-47-3 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester (9CI) (CA INDEX NAME)



RN 343632-48-4 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

L5 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 343632-49-5 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

L5 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

GI

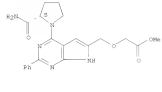
AB Title compds. [I; X1, X2 = N, (substituted) alkyl, aryl, aralkyl; X1X2 = atoms to form (substituted) heterocyclyl; X3 = (substituted) alkyl, aryl, aralkyl; R4 = H, (substituted) alkyl, aryl, aralkyl; R5, R6 = H, halo, (substituted) alkyl, aryl, alkylaryl; R4R5 or R5R6 = (substituted) heterocyclyl, carboxylyl], were prepared Thus, 2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-ylamine and histamine were heated at 110° in MeCN for 6 5 h to give 63% [2-(3H-imidazol-4-yl)ethyl][2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]amine. The latter had 10 times the A3 receptor binding affinity of a reference compound
REFERENCE COUNT: 139 THERE ARE 139 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

L5 ANSWER 11 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:174478 CAPLUS
DOCUMENT NUMBER: 138:221599
TITLE: Preparation of pyrrolo[2,3-d]pyrimidinamines as selective adenosine A1 receptor inhibitors for treatment of asthma, COPD, and other conditions
INVENTOR(S): Castelhano, Arlindo L.; Hofmeister, Bryan; Witter, David J.
PATENT ASSIGNEE(S): GBI Pharmaceuticals, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 79 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003045536	A1	20030306	US 2001-280	20011130
US 6890924	B2	20040510		
US 2004082599	A1	20040429	US 2003-718280	20031120
US 2004082599	A1	20040429	US 2003-718411	20031120
PRIORITY APPLN. INFO.:			US 2000-250895P	P 20001201
			US 2001-280	A1 20011130

OTHER SOURCE(S): MARPAT 138:221599
IT 343632-45-53, (S)-[[4-[2-Carbamoylpyrrolidin-1-yl)-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl]methoxy]acetic acid methyl ester
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(A1 receptor inhibitor; preparation of pyrrolopyrimidinamines adenosine A1 receptor inhibitors from aminocyanopyrroles for treatment of asthma, COPD, and other conditions)
RN 343632-45-5 CAPLUS
CN Acetic acid, [[4-[(2S)-2-[aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-6-yl]methoxy]-, methyl ester (9CI) (CA INDEX NAME)

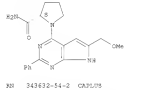
Absolute stereochemistry.



L5 ANSWER 11 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

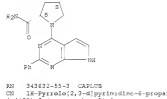
RN 343632-53-1 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-(methoxymethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



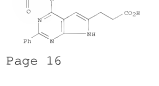
RN 343632-54-2 CAPLUS
CN 2-Pyrrolidinecarboxamide, 4-hydroxy-1-[2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-55-3 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-propanoic acid, 4-[(2S)-2-[aminocarbonyl]-1-pyrrolidinyl]-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

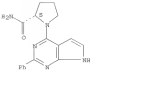


L5 ANSWER 11 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 343631-98-1P, 4-[3-[Acetamido)piperidinyl]-5,6-dimethyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidine 343632-52-0P 343632-53-1P 343632-54-2P 343632-55-3P 343632-57-5P 343632-58-6P 343632-59-7P, 3-(6-Methyl-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl)-(S)-pyrrolidine-2-carboxylic acid amide 343632-60-0P, (S)-1-[6-[(2-Hydroxyethoxy)methyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]pyrrolidine-2-carboxylic acid amide 343632-44-4P, (S)-[[4-[2-Carbamoylpyrrolidin-1-yl)-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl]methoxy]acetic acid 500176-97-2P, (S)-1-[4-[(6-Hydroxy-6-phenylpiperidin-1-yl)methyl]-2-phenyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]pyrrolidine-2-carboxylic acid amide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(A1 receptor inhibitor; preparation of pyrrolopyrimidinamines adenosine A1 receptor inhibitors from aminocyanopyrroles for treatment of asthma, COPD, and other conditions)
RN 343631-98-1 CAPLUS
CN Acetamide, N-[1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-3-piperidinyl]- (9CI) (CA INDEX NAME)

RN 343632-52-0 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S)- (9CI) (CA INDEX NAME)

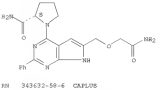
Absolute stereochemistry.



L5 ANSWER 11 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

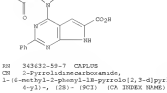
RN 343632-57-5 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-[(2-amino-2-oxoethoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



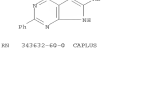
RN 343632-58-6 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(2S)-2-[aminocarbonyl)-1-pyrrolidinyl]-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-59-7 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-60-0 CAPLUS

L5 ANSWER 21 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-pyrrolidinecarboxamide, 1-[4-[[2-hydroxyethoxy)methyl]-2-phenyl-1H-pyrrole]2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

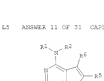
Absolute stereochemistry.

RN 343632-46-6 CAPLUS
CN Acetic acid, [[4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrole]2,3-d]pyrimidin-4-yl]methoxy]- (9CI) (CA INDEX NAME)

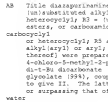
Absolute stereochemistry.

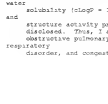
RN 5QG776-87-2 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-[[4-hydroxy-4-phenyl-1-piperidinyl]methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 11 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)





AB Title diazapurinanes I [wherein R1, R2, and R4 = independently H or (un)substituted alkyl(aryl) or aryl; or NR1R2 = (un)substituted heterocyclyl; R3 = (un)substituted alkyl(aryl), aryl, CO2R, carboxy esters, or carbonamides; or C2R3R4 = (un)substituted carbocyclyl or heterocyclyl; R5 and R6 = independently H, halo, or (un)substituted alkyl(aryl) or aryl; and pharmaceutically acceptable salts and prodrugs thereof] were prepared as adenosine A2 specific inhibitors. For example, 4-chloro-5-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidine was protested with di-t-Bu dimethemate (81%), brominated (91%), coupled with anhydrous Me glycolate (93%), coupled with L-prolinamide (92%), and deprotected (93%) to give II. The latter exhibited adenosine A1 receptor binding equal to or surpassing that of reference compds. and is expected to have better water solubility (cLogP = 1.8) than reference compds. (cLogP = 3.8). Efficacy and structure activity profiles of diazapurines of the invention are also disclosed. Thus, I are useful for the treatment of asthma, chronic obstructive pulmonary disease (COPD), allergic rhinitis, upper respiratory disorder, and congestive heart failure (no data).

L5 ANSWER 11 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 343632-56-6P 343633-10-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of pyrrolopyrimidinamines adenosine A1 receptor inhibitors from aminocyanopyrroles for treatment of asthma, COPD, and other conditions)
RN 343632-56-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-carboxylic acid, 4-[(2S)-2-[aminocarbonyl)-1-pyrrolidinyl]-4-[[2-methoxy-2-oxoethoxy)methyl]-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343633-10-3 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-propanoic acid, 4-[(2S)-2-[aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

GI

L5 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:555495 CAPLUS
DOCUMENT NUMBER: 137:109485
TITLE: Preparation of pyrrolopyrimidinylprolineamides and analogs as adenosine receptor antagonists
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Wittar, David J.
PATENT ASSIGNEE(S): Gel Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 308 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057267	A1	20020725	WO 2001-US45280	20011130
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, ZW
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, EW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
US 2002055667	A1	20020516	US 2000-728316	20001201
US 6660722	B2	20040120		
US 2002094974	A1	20020718	US 2000-728616	20001201
US 7160890	B2	20070109		
US 2003036545	A1	20030220	US 2000-728607	20001201
US 6664252	B2	20031216		
CA 2430577	A1	20020725	CA 2001-2430577	20011130
EP 1347980	A1	20031001	EP 2001-997029	20011130
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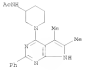
BR 2001015847	A	20040223	BR 2001-15847	20011130
JP 2004517894	T	20040617	JP 2002-558744	20011130
NO 20040892	A2	20040728	NO 2004-892	20011130
NZ 525885	A	20050128	NZ 2001-525885	20011130
IN 2003MN00802	A	20070112	IN 2003-MN802	20030522
NO 20030492	A	20030728	NO 2003-492	20030602
PRIORITY APPLN. INFO.:			US 1999-169037P	P 19991202
			US 2000-728316	A 20001201
			US 2000-728616	A 20001201
			US 2000-728607	A 20001204
			US 1999-169803P	P 19991202
			US 1999-169036P	P 19991202
			WO 2001-US45280	W 20011130

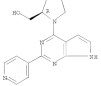
OTHER SOURCE(S): MARPAT 137:109485

L5 ANSWER 33 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 343631-98-3P 343632-22-4P 343632-23-5P
343632-24-6P 343632-25-7P 343632-26-8P
343632-27-9P 343632-28-0P 343632-29-1P
343632-34-8P 343632-42-8P 343632-47-3P
343632-48-4P 343632-49-5P 343632-51-9P
343632-52-0P 343632-53-1P 343632-54-2P
343632-55-3P 343632-57-5P 343632-58-6P
343632-59-7P 343632-60-0P 343632-65-5P
343637-44-6P 343632-48-9P 343637-24-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrrolopyrimidinylprolinexamides and analogs as adenosine
receptor antagonists)
RN 343632-98-1 CAPLUS
CN Acetamide,
N-[1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-3-
piperidinyl]- (9CI) (CA INDEX NAME)

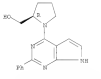


RN 343632-22-4 CAPLUS
CN 2-Pyrrolidinemethanol,
1-[2-(4-pyridinyl)-7H-pyrrolo[2,3-d]pyrimidin-4-yl]-
, (2R)- (9CI) (CA INDEX NAME)

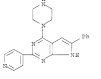
Absolute stereochemistry.



L5 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

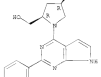


RN 343632-24-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 6-phenyl-4-[3-piperazinyl)-2-(4-pyridinyl)-
(9CI) (CA INDEX NAME)



RN 343631-27-9 CAPLUS
CN 2-Pyrrolidinemethanol, 4-hydroxy-1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-
d]pyrimidin-4-yl]-, (2R,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

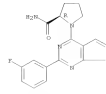


RN 343632-28-0 CAPLUS
CN Alanine, N-[[4-[(2R)-2-(hydroxymethyl)-1-pyrrolidinyl]-2-phenyl-1H-
pyrrolo[2,3-d]pyrimidin-6-yl]methyl]-2-methyl-, methyl ester (9CI) (CA
INDEX NAME)

L5 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

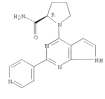
RN 343632-23-5 CAPLUS
CN 2-Pyrrolidinecarboxamide,
1-[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-
4-yl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-24-6 CAPLUS
CN 2-Pyrrolidinecarboxamide,
1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-
yl]-, (2R)- (9CI) (CA INDEX NAME)

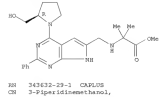
Absolute stereochemistry.



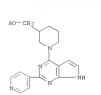
RN 343632-25-7 CAPLUS
CN 2-Pyrrolidinemethanol, 1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-,
(2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

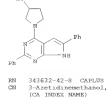
L5 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Absolute stereochemistry.



RN 343632-29-1 CAPLUS
CN 3-Piperidinemethanol,
1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-
(9CI) (CA INDEX NAME)



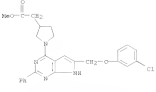
RN 343632-34-8 CAPLUS
CN 3-Pyrrolidinol, 1-(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)- (9CI)
(CA INDEX NAME)



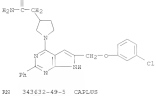
RN 343632-42-8 CAPLUS
CN 3-Azetidinemethanol, 1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)- (9CI)
(CA INDEX NAME)

L5 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343632-47-3 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-3H-pyrrolo[3,4-d]pyrimidin-4-yl]-, methyl ester (9CI) (CA INDEX NAME)



RN 343632-48-4 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[3,4-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)



RN 343632-49-5 CAPLUS
CN 3-Pyrrolidinemethanol, 1-[4-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[3,4-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

L5 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry.

RN 343632-54-2 CAPLUS
CN 2-Pyrrolidinecarboxamide,
4-hydroxy-1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S,4R)- (9CI) (CA INDEX NAME)

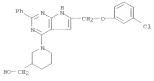
Absolute stereochemistry.

RN 343632-55-3 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-propanoic acid,
4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

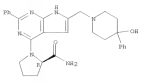
RN 343632-57-5 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-[(2-amino-2-oxoethoxy)methyl]-2-phenyl-1H-pyrrolo[3,4-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

L5 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



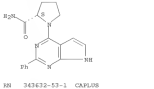
RN 343632-51-9 CAPLUS
CN 2-Pyrrolidinecarboxamide,
1-[6-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-52-0 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S)- (9CI) (CA INDEX NAME)

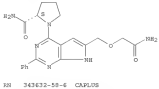
Absolute stereochemistry.



RN 343632-53-1 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-(methoxymethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

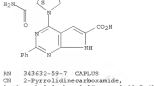
L5 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry.



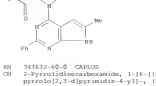
RN 343632-58-6 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid,
4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-59-7 CAPLUS
CN 2-Pyrrolidinecarboxamide,
1-(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-60-0 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-[(2-hydroxyethoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343632-65-5 CAPLUS
CN Acetic acid, [[4-[[2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[3,4-d]pyrimidin-6-yl]methoxy]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-66-6 CAPLUS
CN Acetic acid, [[4-[(2S)-2-[aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[3,4-d]pyrimidin-6-yl]methoxy]- (9CI) (CA INDEX NAME)

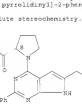
Absolute stereochemistry.

RN 343632-68-8 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[4-[3-methoxyphenyl]-2-(4-pyridinyl)-1H-pyrrolo[3,4-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAME)

L5 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343633-10-3 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-4-propanoic acid, 6-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI

AB Title compds., e.g., I, were prepared Data for biol. activity of title compds. were given.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 12 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Absolute stereochemistry.

RN 343633-24-9 CAPLUS
CN 2-Pyridinemethanamine, 1-[6-phenyl-2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 343632-56-4P 343633-10-3P
RLs RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrrolopyrimidinylprolinesamides and analogs as adenosine
receptor antagonists)
RN 343632-56-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-carboxylic acid, 4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-6-[[2-methoxy-2-oxoethoxy)methyl]-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:540257 CAPLUS
DOCUMENT NUMBER: 137:109288
TITLE: Preparation of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A3 receptor
INVENTOR(S): Castilhano, Arlindo L.; McKibben, Bryan; Witter, David J.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 87 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002094974	A1	20020718	US 2000-728616	20001201
US 7160890	B2	20070109		
CA 2430577	A1	20020725	CA 2001-2430577	20011130
WO 2002057267	A1	20020725	WO 2001-US45280	20011130
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1347989	A1	20031001	EP 2001-987828	20011130
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001015847	A	20040225	BR 2001-15847	20011130
JP 2004517896	T	20040617	JP 2002-557944	20011130
MX 2004006692	A2	20040728	MX 2004-692	20011130
NO 5258/05	A	20050128	NO 2003-5258/05	20011130
NO 2003002482	A	20030728	NO 2003-2482	20030602
PRIORITY APPLN. INFO.:			US 1999-169036P	P 19991202
			US 1999-169037P	P 19991202
			US 2000-728316	A 20001201
			US 2000-728697	A 20001201
			US 2000-728616	A 20001201
			WO 2001-US45280	W 20011130

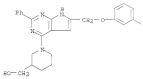
OTHER SOURCE(S): MARPAT 137:109288
IT 053946-53-9P 343632-24-8P 343632-42-8P 343632-47-3P 343632-48-4P 343632-49-5P 343632-84-8P 343632-85-9P 343632-86-0P 343632-87-1P 343632-88-2P 343632-89-3P 343632-90-6P 343969-99-2P 443118-20-5P 443118-74-9P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

L5 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(invention compd., prepn. of pyrrolo[2,3-d]pyrimidines as selective inhibitors of the adenosine A3 receptor for the treatment of diseases such as diarrhea, allergic rhinitis, and eye damage resulting from injuries or disease)
RN 251946-03-9 CAPLUS
CN Acetamide, N-[1-(5,6-dimethyl-7-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-4-piperidinyl]- (9CI) (CA INDEX NAME)

RN 343632-34-8 CAPLUS
CN 3-Pyrrolidinol, 1-[2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

RN 343632-42-8 CAPLUS
CN 3-Azetidinemethanol, 1-[2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

L5 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 343632-84-8 CAPLUS
CN 3-Pyrrolidinol, 1-[2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

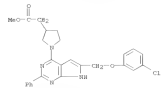
RN 343632-85-9 CAPLUS
CN 3-Pyrrolidinol, 1-[2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

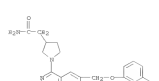
RN 343632-86-0 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester, (3R)- (9CI) (CA INDEX NAME)

L5 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343632-47-3 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester (9CI) (CA INDEX NAME)



RN 343632-48-4 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)



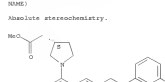
RN 343632-49-5 CAPLUS
CN 3-Pyrrolidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

L5 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry.

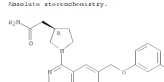
RN 343632-87-1 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-88-2 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3S)- (9CI) (CA INDEX NAME)

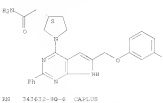
Absolute stereochemistry.



RN 343632-89-3 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3R)- (9CI) (CA INDEX NAME)

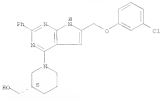
L5 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry.



RN 347672-90-6 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[[3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[3,7-d]pyrimidin-4-yl]-, (3S)- (9CI) (CA INDEX NAME)

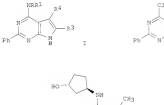
Absolute stereochemistry.



RN 343969-98-2 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[[3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[3,2-d]pyrimidin-4-yl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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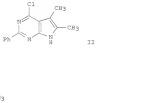

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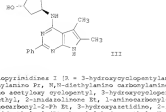
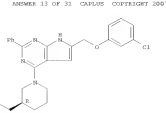


III

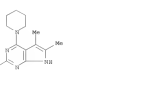
AB Pyrrolopyrimidines I [R = 3-hydroxycyclopentylamino ethylamino carbonylamino Pr, N,N-diethylamino carbonylamino Et, thioacetamido Et, 3-amino acetyloxy cyclopentyl, 3-hydroxycyclopentyl, 2-pyrrolyl carbonyl aminoethyl, 2-imidazolineoxe Et, 1-anilocarbonyl-2-methylpropyl, 1-aminocarbonyl-2-Ph Et, 3-hydroxyacetidino, 2-imidazolethyl, acetamidomethyl, 1-(3)-phenyl-2-hydroxyethyl, N-methylaminocarbonyl pyridyl-2-methyl; R1 = H; R2R3 = 3-hydroxypyrrolidino, 3-methyloxy carbonylethyl pyrrolidino, 3-aminocarbonylmethyl pyrrolidino, 3-hydroxymethyl piperidino; R3, R4 = H, (un)substituted alkyl, aryl] are prepared as selective inhibitors of adenosine receptors, particularly the adenosine A3 receptor, for the treatment of diseases such as asthma, diarrhea, chronic obstructive pulmonary disease, allergic rhinitis, or for the treatment of eye damage caused either by disease or injury. Human adenosine receptors are transformed into yeast; the modified yeast are used to assay the invention compds. I for their adenosine receptor binding and selectivities. E.g., 2-(1-phenylethyl)-2-amino-3-cyano-4,5-dimethylpyrrole is acylated with PhCOCl to give the benzamide which undergoes cyclocondensation with concentrated H2SO4 in MeOH to give a pyrrolopyrimidinone; removal of the phenethyl group with polyphosphoric acid and chlorination of the pyrrolopyrimidinone with POCl3 gives the intermediate chloropyrrolopyrimidine II. E.g., addition of amines such as trans-3-amino-1-cyclopentanol to II in DMSO gives aminopyrrolopyrimidines such as III. III has a Ki for the adenosine A1 receptor of 29 nM and a Ki for the adenosine A3 receptor of 3.1 nM while binding to the adenosine A2a and A2b receptors with Ki values of 191 nM and 1143 nM, resp. Formulations of these compds. are claimed (no data). Methods for the preparation of I from the acylation of aminopyrroles with acyl chlorides followed by cyclocondensation and deprotection, chlorination, and substitution of the chlorine atom with an amine are claimed.
REFERENCE COUNT: 129 THERE ARE 129 CITED REFERENCES AVAILABLE FOR

L5 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 443118-20-5 CAPLUS
CN 3-Azetidinemethanol, 1-[2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

RN 443118-74-9 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 5,6-dimethyl-2-phenyl-4-(1-piperidinyl)- (9CI) (CA INDEX NAME)



GI

L5 ANSWER 13 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:369892 CAPLUS
DOCUMENT NUMBER: 136:386128
TITLE: Synthesis and use of substituted pyrrolo[2,3-b]pyridines as selective adenosine A1, A2a and A3 receptor antagonists
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
PATENT ASSIGNEE(S): GPI Pharmaceuticals, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 79 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20020058667	A1	20020516	US 2000-728316	20001201
US 6492322	B2	20041220		
CA 2409177	A1	20020725	CA 2001-2409177	20011130
WO 2002057287	A1	20020725	WO 2001-US45280	20011130
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1347980	A2	20031001	EP 2001-997029	20011130
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, LT, LV, RO, MK, CY, AL, TR				
BR 2001015847	A	20040225	BR 2001-15847	20011130
JP 2004517096	T	20040617	JP 2002-557944	20011130
NO 20040692	A2	20040728	NO 2004-692	20011130
NO 325895	B	20080128	NO 2003-2585	20011130
ZA 2003003729	A	20040514	ZA 2003-3729	20030514
IN 2003DN00502	A	20070112	IN 2003-DN502	20030522
NO 20032492	A	20030728	NO 2003-2492	20030602
PRIORITY APPLN. INFO.:			US 1999-169037P	P 19991202
			US 2000-728316	A 20001201
			US 2000-728607	A 20001201
			US 2000-728616	A 20001201
			WO 2001-US45280	W 20011130

OTHER SOURCE(S): MARPAT 136:386128

L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 343633-90-3P, Acetamide, N-(1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-3-piperidinyl)- 343632-48-8P, Propanamide, 2-amino-N-[1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-4-piperidinyl]- 343632-22-4P, 2-Pyrrolidinecarboxamide, 1-[6-[4-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-3-piperidinyl]- 343632-23-5P, 2-Pyrrolidinecarboxamide, 1-[2-[4-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- 343632-24-6P, 2-Pyrrolidinecarboxamide, 1-[2-[4-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- 343632-25-7P, 2-Pyrrolidinemethanol, 1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2R)- 343632-26-8P, 1H-Pyrrolo[2,3-d]pyrimidine, 6-phenyl-4-(1-piperazinyl)-2-(4-pyridinyl)- 343632-27-9P, 2-Pyrrolidinemethanol, 1-hydroxy-1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R,4S)- 343632-28-0P, Alanine, N-[[4-[(2R)-2-(hydroxymethyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-6-yl]methyl]-2-methyl-, methyl ester 343632-29-1P, 3-Piperidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- 343632-51-9P, 2-Pyrrolidinecarboxamide, 1-[6-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- 343632-52-0P, 2-Pyrrolidinecarboxamide, 1-[6-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- 343632-53-1P, 2-Pyrrolidinecarboxamide, 1-[6-[methoxymethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- 343632-54-2P, 2-Pyrrolidinecarboxamide, 4-hydroxy-1-[2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S,4R)- 343632-55-3P, 1H-Pyrrolo[2,3-d]pyrimidine-6-propanoic acid, 4-[(2S)-2-[(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl- 343632-57-5P, 2-Pyrrolidinecarboxamide, 1-[6-[(2-amino-2-oxoethoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- 343632-58-6P, 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(2S)-2-[aminocarbonyl)-1-pyrrolidinyl]-2-phenyl- 343632-59-7P, 2-Pyrrolidinecarboxamide, 1-[6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- 343632-60-0P, 2-Pyrrolidinecarboxamide, 1-[6-[(2-hydroxyethoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- 343632-65-5P, Acetic acid, [[4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-6-yl]methoxy]-, methyl ester 343632-66-6P, Acetic acid, [[4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-6-yl]methoxy]- 343632-67-7P, 2-Pyrrolidinecarboxamide, 1-[6-[[3-methoxyphenyl)-2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (2S)- 343632-74-6P, 3-Piperidinemethanol, 1-[3-[4-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (3S)- 343632-75-7P, 3-Piperidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3R)- 343632-84-6P, 3-Pyrrolidinol, 1-(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (3R)- 343632-85-8P, 3-Pyrrolidinol, 1-(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (3S)- 343632-86-0P, 3-Pyrrolidinesetic acid, 1-[6-[(1-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester, (3R)- 343632-87-1P, 3-Pyrrolidinesetic

L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester, (3R)- 343632-88-2P, 3-Pyrrolidinesetamide,

1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3S)- 343632-89-3P, 3-Pyrrolidinesetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3S)- 343632-90-6P, 3-Piperidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3R)- 343633-24-9P, 2-Pyrrolidinecarboxamide, 1-[6-phenyl-2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- 343969-98-2P, 3-Piperidinemethanol,

1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3R)-
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preps. and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A1, A2a and A3 receptor antagonists)

RN 343633-98-1 CAPLUS
CN Acetamide, N-[1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-3-piperidinyl]- (9CI) (CA INDEX NAME)

RN 343632-18-8 CAPLUS
CN Propanamide, 2-amino-N-[1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-4-piperidinyl]- (9CI) (CA INDEX NAME)

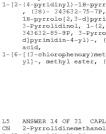
RN 343632-22-4 CAPLUS

L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Pyrrolidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- , (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

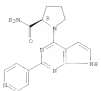
RN 343632-23-5 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



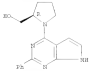
RN 343632-24-6 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

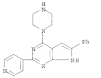


RN 343632-25-7 CAPLUS
CN 2-Pyrrolidinemethanol, 1-[2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

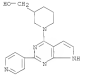
Absolute stereochemistry.



RN 343632-26-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 6-phenyl-4-(1-piperazinyl)-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)

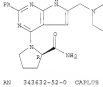


RN 343632-27-9 CAPLUS
CN 2-Pyrrolidinemethanol, 4-hydroxy-1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S,4R)- (9CI) (CA INDEX NAME)



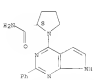
RN 343632-51-9 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[4-[4-hydroxy-4-phenyl-1-piperidinyl]methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-52-0 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S)- (9CI) (CA INDEX NAME)

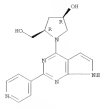
Absolute stereochemistry.



RN 343632-53-1 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-(methoxymethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

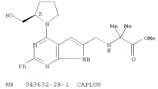
Absolute stereochemistry.

Absolute stereochemistry.

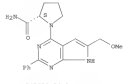


RN 343632-28-0 CAPLUS
CN Alanine, N-[[4-[(2S)-2-(hydroxymethyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-6-yl]methyl]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

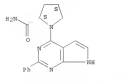


RN 343632-29-1 CAPLUS
CN 3-Piperidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)



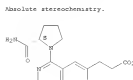
RN 343632-54-2 CAPLUS
CN 2-Pyrrolidinecarboxamide, 4-hydroxy-1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-55-3 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-propanoic acid, 4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-57-5 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-[[2-amino-2-oxoethoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343632-58-6 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-6-ylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

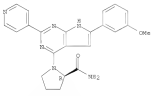
RN 343632-59-7 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-60-0 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-[[2-hydroxyethoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry.



RN 343632-74-6 CAPLUS
CN 3-Piperidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-73-7 CAPLUS
CN 3-Piperidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry.

RN 343632-65-5 CAPLUS
CN Acetic acid, [[4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-6-yl]methoxy]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-66-6 CAPLUS
CN Acetic acid, [[4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-6-yl]methoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-68-8 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-(3-methoxyphenyl)-2-(4-pyridinyl)-1H-

L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343632-84-8 CAPLUS
CN 3-Pyrrolidinol, 1-(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

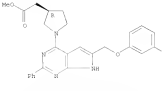
RN 343632-85-9 CAPLUS
CN 3-Pyrrolidinol, 1-(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-86-0 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-

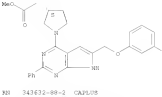
L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-87-1 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

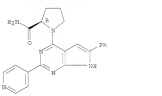


RN 343632-88-2 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

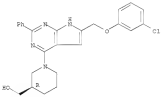
L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 343633-24-9 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-phenyl-2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343969-98-2 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3R)- (9CI) (CA INDEX NAME)

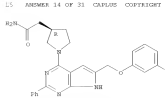
Absolute stereochemistry.



IT 343632-86-4P, 7H-Pyrrolo[2,3-d]pyrimidine-7-carboxylic acid, 4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-6-[(2-methoxy-2-oxoethoxy)methyl]-2-phenyl-, 1,1-dimethylethyl ester 343633-10-2P, 1H-Pyrrolo[2,3-d]pyrimidine-6-propanoic acid, 4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-, 1,1-dimethylethyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and use of substituted 7H-pyrrolo[2,3-b]pyrimidines as selective adenosine A1, A2a and A3 receptor antagonists)
RN 343632-56-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-carboxylic acid, 4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-6-[(2-methoxy-2-oxoethoxy)methyl]-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

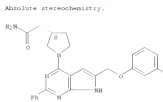
Absolute stereochemistry.

L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



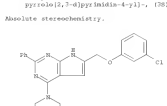
RN 343632-89-3 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-90-6 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

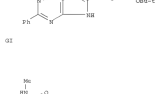


L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343633-10-3 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-6-propanoic acid, 4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

GI



I II

L5 ANSWER 14 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
AB Title compds. I and analogs [R2 = 5-6 membered aromatic ring; R3-4 = H, alkyl] were prepared. Over 300 examples were provided. Intermediate 4-chloro-7H-pyrrolo[2,3-d]pyrimidines were prepared by several routes from appropriately substituted cyano-pyrroles. Thus, 4-chloro-3-(4-pyridyl)-7H-pyrrolo[2,3-d]pyrimidine hydrochloride was reacted with D-prolinol (2.3 mol equiv) in DMSO at 125° for 18 h to yield II in 13% yield after purification. Compound I [R2 = Ph; R3-4 = Me] exhibited 10-fold selectivity for histidine to the adenosine A1 receptor than to A2a, A2b or A3 receptors. Ki values were determined for selected example compds. I are useful for the treatment of COPD, allergic rhinitis, etc.

L5 ANSWER 15 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:747994 CAPLUS
DOCUMENT NUMBER: 136:134733
TITLE: Synthesis of several isotopically labeled pyrrolo[3,7-d]pyrimidine analogs
AUTHOR(S): Easter, John A.; Stoilo, Wayne T.
CORPORATE SOURCE: Global Drug Metabolism, Pharmacia Corporation, Kalamazoo, MI, 49007, USA
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (2001), 44(11), 797-810
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: John Wiley & Sons Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:134731
IT 392245-85-1P 392245-91-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isotopically labeled pyrrolopyrimidines)
RN 392245-85-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-2-14C, 7-methyl-4-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

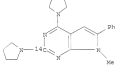
RN 392245-91-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-2-14C, 6,7-dimethyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

IT 392245-86-2P 392245-87-3P

L5 ANSWER 15 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of isotopically labeled pyrrolopyrimidines)
RN 392245-86-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-2-14C, 7-methyl-4-phenyl-2,4-di-1-pyrrolidinyl- , monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 392245-85-1
CMF C21 H25 N5



CM 2

CRN 75-75-2
CMF C H4 O3 S

L5 ANSWER 15 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

● HCl

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Four members of a novel class of pyrrolo[2,3-d]pyrimidines that show potential for the treatment of asthma and neurodegenerative disorders, have been prepared with radioisotope labels and in one case with multiple stable isotope labels for ADME studies as part of the drug development process. The syntheses utilize an isotopically labeled 2,4,6-trisubstituted pyrimidine as a common building block, readily prepared from isotopically labeled urea. Cyclizations of the pyrimidine with bromo-ketones generate the ring fused pyrrolo[2,3-d]-pyrimidines with elegant efficiency as demonstrated by the preparation of structures I (R = Ph, Me) as the mesylate or HCl salt, resp., II, and III (X = 12C, Y = 14C, Z = 14N; X = Y = 13C, Z = 15N) as the HCl salts.
REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:416773 CAPLUS
DOCUMENT NUMBER: 135:46190
TITLE: Synthesis and use of substituted pyrrolo[2,3-b]pyridines as selective adenosine A1, A2a and A3 receptor antagonists
INVENTOR(S): Castelhano, Arlindo L.; McAbbeen, Bryan; Witter, David J.
PATENT ASSIGNEE(S): Gai Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 368 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002039977	A1	20020607	WO 2000-US31702	20001201
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6686766	B1	20040203	US 1999-454075	19991202
US 6878736	B2	20050412	US 1999-454074	19991202
CA 2393179	A1	20010607	CA 2000-2393179	20001201
EP 1246623	A1	20021009	EP 2000-988011	20001201
EP 1246623	B1	20060809		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003533502	T	20031107	JP 2001-541509	20001201
AU 784878	B2	20060713	AU 2001-24270	20001201
PRIORITY APPLN. INFO.:			US 1999-454074 A	19991202
			US 1999-454075 A	19991202
			US 1999-454254 A	19991202
			US 1998-87702P P	19980602
			US 1999-123216P P	19990308
			US 1999-126527P P	19990326
			WO 1999-US12135 A2	19990601
			WO 2000-US31702 W	20001201

OTHER SOURCE(S): MARPAT 135:46190

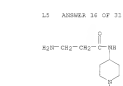
L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343632-22-4 CAPLUS
CN 2-Pyrrolidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAMES)

Absolute stereochemistry.

RN 343632-23-5 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[2-(3-fluorophenyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAMES)

Absolute stereochemistry.



L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 343633-98-1P 343632-18-8P 343632-22-4P
343632-23-5P 343632-24-6P 343632-25-7P
343632-26-8P 343632-27-9P 343632-28-0P
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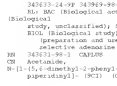
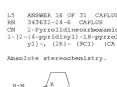
343632-47-3P 343632-48-4P 343632-49-5P
343632-51-9P 343632-52-0P 343632-53-1P
343632-54-2P 343632-55-3P 343632-57-5P
343632-58-6P 343632-59-7P 343632-60-0P
343632-65-5P 343632-66-6P 343632-68-8P
343632-74-4P 343632-75-5P 343632-84-8P
343632-85-9P 343632-86-0P 343632-87-1P
343632-88-2P 343632-89-3P 343632-90-6P
343633-24-9P 343639-99-2P
(unclassified; BSU (Biological study, unclassified); EXS (Exploratory study, unclassified); FMU (Formulation, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and use of substituted 7H-pyrrolo[2,3-d]pyrimidines as selective adenosine A1, A2a and A3 receptor antagonists)
RN 343631-98-1 CAPLUS
CN Acetamide, N-[1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-3-piperidinyl]- (9CI) (CA INDEX NAMES)



RN 343632-18-8 CAPLUS
CN Propanamide, 3-amino-N-[1-(5,6-dimethyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-4-piperidinyl]- (9CI) (CA INDEX NAMES)

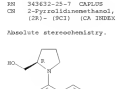
RN 343632-22-4 CAPLUS
CN 2-Pyrrolidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAMES)

Absolute stereochemistry.

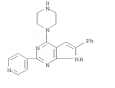


RN 343632-23-5 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[2-(3-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2R)- (9CI) (CA INDEX NAMES)

Absolute stereochemistry.



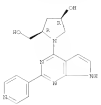
RN 343632-26-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 6-phenyl-4-(3-piperazinyl)-2-(4-pyridinyl)- (9CI) (CA INDEX NAMES)



RN 343632-27-9 CAPLUS

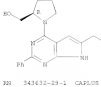
L5 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 2-Pyrrolidinemethanol, 4-hydroxy-1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S,4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-28-0 CAPLUS
CN Alanine, N-[[4-[(2R)-2-(hydroxymethyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[3,2-d]pyrimidin-6-yl]methyl]-2-methyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-29-1 CAPLUS
CN 3-Piperidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

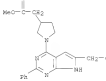
L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343632-34-8 CAPLUS
CN 3-Pyrrolidinol, 1-(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)- (9CI) (CA INDEX NAME)

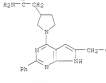
RN 343632-42-8 CAPLUS
CN 3-Azetidinemethanol, 1-[2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

RN 343632-47-3 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester (9CI) (CA INDEX NAME)

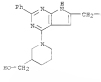
L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 343632-48-4 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)



RN 343632-49-5 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)



RN 343632-51-9 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-[(4-hydroxy-4-phenyl-1-piperidinyl)methyl]-2-phenyl-1H-pyrrolo[3,2-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 343632-52-0 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-(2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 343632-53-1 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-(methoxymethyl)-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

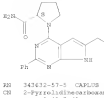
RN 343632-54-2 CAPLUS
CN 2-Pyrrolidinecarboxamide, 4-hydroxy-1-[2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S,4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

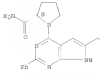
RN 343632-55-3 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-4-propanoic acid, 4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



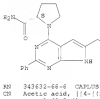
RN 343632-57-5 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[4-[[2-amino-2-oxoethoxy]methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



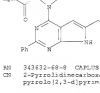
RN 343632-58-6 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine-4-carboxylic acid, 4-[(2S)-2-(aminocarbonyl)-1-

L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



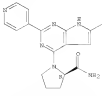
RN 343632-66-6 CAPLUS
CN Acetic acid, [[4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]methoxy]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-68-8 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-(3-methoxyphenyl)-2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2R)- (9CI) (CA INDEX NAME)

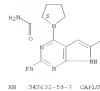
Absolute stereochemistry.



RN 343632-74-6 CAPLUS
CN 3-Pyperidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-

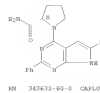
L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
pyrrolidinyl]-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



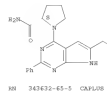
RN 343632-59-7 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-(6-methyl-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-60-0 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-[[2-hydroxyethoxy]methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

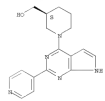
Absolute stereochemistry.



RN 343632-65-5 CAPLUS

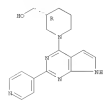
L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-75-7 CAPLUS
CN 3-Pyperidinemethanol, 1-[2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrinidin-4-yl]-, (3R)- (9CI) (CA INDEX NAME)

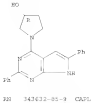
Absolute stereochemistry.



RN 343632-84-8 CAPLUS
CN 3-Pyrrolidinol, 1-(2,6-diphenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl)-, (3R)- (9CI) (CA INDEX NAME)

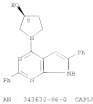
Absolute stereochemistry.

L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



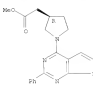
RN 343632-85-9 CAPLUS
CN 3-Pyrrolidino[, 1-1],6-diphenyl-1H-pyrrolo[3,4-d]pyrimidin-4-yl)-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

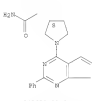


RN 343632-86-0 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

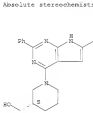


L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



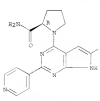
RN 343632-90-6 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343633-24-9 CAPLUS
CN 2-Pyrrolidinecarboxamide, 1-[6-phenyl-2-(4-pyridinyl)-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

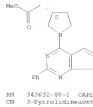


RN 343969-98-2 CAPLUS
CN 3-Piperidinemethanol, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3R)- (9CI) (CA INDEX NAME)

L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

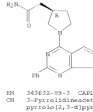
RN 343632-87-1 CAPLUS
CN 3-Pyrrolidineacetic acid, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, methyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 343632-88-2 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

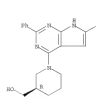


RN 343632-89-3 CAPLUS
CN 3-Pyrrolidineacetamide, 1-[6-[(3-chlorophenoxy)methyl]-2-phenyl-1H-pyrrolo[2,3-d]pyrimidin-4-yl]-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

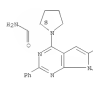
L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Absolute stereochemistry.



IT 343632-56-4P 343633-10-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and use of substituted 7H-pyrrolo[2,3-b]pyridines as selective adenosine A1, A2a and A3 receptor antagonists)
RN 343632-56-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-carboxylic acid, 4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-6-[(2-methoxy-2-oxoethoxy)methyl]-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

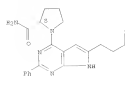
Absolute stereochemistry.



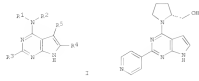
RN 343633-10-3 CAPLUS
CN 1H-Pyrrole[2,3-d]pyrimidine-6-propanoic acid, 4-[(2S)-2-(aminocarbonyl)-1-pyrrolidinyl]-2-phenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



GI



AB The synthesis of compds. I, their binding to adenosine receptors and use are described [wherein R1, R2 = H, (un)substituted alkyl or NR1R2 = (un)substituted 4-8 membered ring; R3 = (un)substituted 4-6 membered (aromatic) ring; R4, R5 = H, (un)substituted alkyl, aryl (with some exceptions)]. Over 100 examples are provided. Intermediate 4-chloro-7H-pyrrolo[2,3-d]pyrimidines were prepared by several routes from
appropriately substituted cyano-pyroles. Thus, 4-chloro-2-(4-pyridyl)-7H-
pyrrolo[2,3-d]pyrimidine hydrochloride was reacted with D-prolinol (2.3 mol equiv) in DMSO at 120°C for 18 h to yield III in 13% yield after purification. Compound I [R1 = AcNHCH2CH2; R2 = H; R3 = Ph; R4, R5 = Me;
II] exhibited selective binding to adenosine receptor A1 with IC50 = 82.8 nM. Compound II also had K1 = 9.8 nM (vs. K1 = 7.1 for control ligand 8-cyclopentyl-1,3-dipropylxanthine (DPCPX)). Pyrimidine III binds 5 times
more selectively to adenosine receptor A2a than A1, A2b or A3 (no data). Compound I [R1 = AcNH(CH2)4; R2 = H; R3 = Ph; R4, R5 = Me] is 10 times more
selective for A3 than the other receptor subtypes. ClogP (calculated partition coefficient between octanol and H2O) values were determined for selected
example compds. Claimed uses of I includes administration of a systemic

L5 ANSWER 16 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
formulation (i.e. ophthalmic) for the treatment of a disease arrocd. with A1, A2a, and A3 adenosine receptors in a subject.
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 17 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN

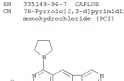
ACCESSION NUMBER: 2001:88379 CAPLUS
DOCUMENT NUMBER: 134:311371
TITLE: Synthesis of 2,4-diaminopyrrolo[2,3-d]pyrimidines via thermal Fischer indolization. Pyrazole formation with ytterbium triflate catalysis
AUTHOR(S): Brady, Gordon L.; Schwartz, Theresa M.; Palmer, John R.; Bamitt, Lee E.; Watt, William
CORPORATE SOURCE: Combinatorial and Medicinal Chemistry, Pharmacia and Upjohn, Kalamazoo, MI, 49001, USA
SOURCE: Journal of Heterocyclic Chemistry (2000), 37(6), 1471-1477
CODEN: JHTCAD; ISSN: 0022-152X
PUBLISHER: HeteroCorporation
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:311371
IT 335149-83-2P 335149-84-3P
RL: SPH (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 335149-83-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-4-pyrazinyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 335149-84-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-4-(4-pyridinyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

IT 157012-18-5P, PMD 87663 335149-96-7P 335149-97-8P
RL: SPH (Synthetic preparation); PREP (Preparation)
(preparation of (amino)pyrrolo[2,3-d]pyrimidines via thermal Fischer indolization and pyrazole formation with ytterbium triflate catalysis)
RN 157012-18-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-4-phenyl-2,4-di-1-pyrrolidinyl-

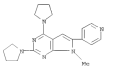
L5 ANSWER 17 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)

RN 335149-96-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-4-pyrazinyl-2,4-di-1-pyrrolidinyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 335149-97-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-4-(4-pyridinyl)-2,4-di-1-pyrrolidinyl-, dihydrochloride (9CI) (CA INDEX NAME)



● 2 HCl

AB The high-yield synthesis of the 2,4-diaminopyrrolo[2,3-d]pyrimidine (PMD-87663) via a Bischler-like alkylation-cyclization sequence was reported earlier. Herein an alternative synthesis of this potent

L5 ANSWER 17 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
antioxidant and several analogs based on the thermal Fischer indolization,
starting from hydrazine substituted pyridinones is described. In several cases where the thermal Fischer indolization failed, attempts to catalyze the reaction with Lewis acids, esp. ytterbium triflate, led to the surprising and unprecedented formation of pyrazolo[3,4-d]pyrimidines, e.g.,
1-methyl-3-phenyl-4,6-di-1-pyrrolidinyl-1H-pyrazolo[3,4-d]pyrimidine, with
the loss of the elements of methane. Mechanistic details of this transformation remain to be investigated. A poln. of 4-(1-methylhydrazino)-2,6-di-1-pyrrolidinylpyrimidine (1.91 mmol), 4-(1-indazolyl)acetophenone (5.59 mmol), ytterbium trifluoromethanesulfonate (0.19 mmol) in decalin (50 mL) was heated at reflux under nitrogen (or 18 h. Removal of solvent and purifn. by chromatog. on silica gel gave
3-(4-(1H-indazol-1-yl)phenyl)-1-methyl-4,6-di-1-pyrrolidinyl-1H-pyrazolo[4,4-d]pyrimidine in 25% yield.
REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

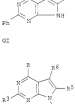
L5 ANSWER 18 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:787837 CAPLUS
DOCUMENT NUMBER: 132:122973
TITLE: Preparation of pyrrolo[2,3-d]pyrimidines as adenosine receptor antagonists
INVENTOR(S): Castelhano, Arlindo L.; McKibben, Bryan; Witter, David J.
PATENT ASSIGNEE(S): Cadus Pharmaceutical Corp., USA
SOURCE: PCT Int. Appl., 169 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9962518	A1	19991209	WO 1999-US12135	19990601
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
CA 2334200	A1	19991209	CA 1999-2334200	19990601
AU 9942265	A	19991220	AU 1999-42265	19990601
AU 767658	B2	20031211		
EP 1091612	A	20010606	EP 1999-11612	19990601
EP 1082129	A1	20010314	EP 1999-926107	19990601
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200003513	T2	20010621	TR 2000-200003513	19990601
HU 2001003836	A2	20020228	HU 2001-3836	19990601
JP 2002516861	T	20020611	JP 2000-551774	19990601
NZ 508314	A	20040326	NZ 1999-508314	19990601
TW 241435	B	20051101	TW 1999-88109694	19990728
US 6486366	B1	20040203	US 1999-414675	19991202
US 6878716	B1	20050412	US 1999-414674	19991202
NO 20006096	A	20010131	NO 2000-6096	20001130
US 2002028782	A1	20020307	US 2000-728229	20001201
US 6806633	B2	20041005		
US 2005043332	A1	20050224	US 2004-816329	20040331

PRIORITY APPLN. INFO.: US 1998-107902P P 19980602
US 1999-123216P P 19990308
US 1999-126527P P 19990326
WO 1999-US12135 W 19990601
US 2000-728229 A3 20001201

L5 ANSWER 19 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
OTHER SOURCE(S): MARPAT 132:122973
IT 251946-53-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrrolo[2,3-d]pyrimidines as adenosine receptor antagonists)
RN 251946-53-9 CAPLUS
CN Acetamide, N-[1-[5,6-dimethyl-2-(1-pyrrolo[2,3-d]pyrimidin-4-yl)-4-piperidinyl]- (9CI) (CA INDEX NAME)

GI



AB Title compds. [I; R = NR1R2; R1-R4 = H, alkyl, aryl, etc.; NR1R2 = heterocephyly; R5,R6 = H, halo, alkyl, aryl, etc.; R4R5,R5R6 = atoms to complete a ring] were prepared This, 2- amino-3-cyano-6,5-dimethyl-1-(1-phenylethyl)pyrrole was N-benzoylated and the product cyclized to give, after deprotection and chlorination, I (R3 = Ph; R4 = H, R5 = R6 = Me);[II; R = Cl] which was animated by trans-4-hydroxycyclohexylamine to give II (R = trans-4-hydroxycyclohexylamino). Data for biol. activity of I were given.
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

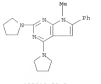
L5 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:166163 CAPLUS
DOCUMENT NUMBER: 130:246769
TITLE: Novel, highly lipophilic antioxidants readily diffuse across the blood-brain barrier and access intracellular sites
AUTHOR(S): Sawada, Geri A.; Williams, Lawrence R.; Lutzke, Barry S.; Raub, Thomas J.
CORPORATE SOURCE: Drug Absorption and Transport, Pharmacia and Upjohn, Inc., Kalamazoo, MI, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (1999), 288(3), 1327-1333
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 157013-18-5, PNU-87663 157013-32-6, PNU 89843
RL: BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(lipophilic pyrrolopyrimidine antioxidants diffusion across blood-brain
barrier and pharmacokinetics in CNS and other tissues)
RN 157013-18-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-4-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 157013-32-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

AB In an accompanying article, an in vitro assay for permeability predicts that membrane-protective, antioxidant 2,4-diamino-pyrrolo[2,3-

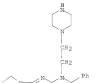
L5 ANSWER 19 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
clpyrimidines should have improved blood-brain barrier (BBB) permeation over previously described lipophilic antioxidants. Using a first-pass exts. method and brain/plasma quantification, we show here that two of the
pyrrolopyrimidines, one of which is markedly less permeable, readily partition into rat brain. The efficiency of exts. was dependent on serum protein binding, and in situ efflux confirms the in vitro data showing that PNU-87663 is retained in brain longer than PNU-87643. By exploiting inherent fluorescence properties of PNU-87663, its distribution within brain and within cells in culture was demonstrated using confocl scanning
laser microscopy. PNU-87663 rapidly partitioned into the cell membrane and equilibrated with cytoplasmic compartments via passive diffusion. Although partitioning of PNU-87663 favors intracytoplasmic lipid storage droplets, the compd. was readily exchangeable as shown by efflux of compd.
from cells to buffer when protein was present. The results demonstrated that pyrrolopyrimidines were well suited for quickly accessing target cells within the central nervous system as well as in other target tissues.
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:166121 CAPLUS
DOCUMENT NUMBER: 131:181
TITLE: Increased lipophilicity and subsequent cell partitioning decrease passive transcellular diffusion of novel, highly lipophilic antioxidants
AUTHOR(S): Kawada, Seti A.; Harsahu, Craig L.; Lohse, Barry S.; Houghton, Michael E.; Padbury, Guy S.; Ho, Norman F. H.; Raub, Thomas J.
CORPORATE SOURCE: Drug Absorption and Transport, Pharmacia and Upjohn, Inc., Kalamazoo, MI, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (1999), 288(1), 1317-1326
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: American Society for Pharmacology and Experimental Therapeutics
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 157012-18-5 157012-32-3 157012-34-5
157012-38-9 157012-41-4 157012-46-9
157012-47-0 157012-48-1 157012-56-1
157012-58-3 157012-61-8 157012-75-4
157012-84-5 157012-85-6 157012-89-0
157012-90-3 157012-91-4 157013-30-4
157013-31-5 157013-32-6 157013-33-7
157013-34-8 225115-52-6 225115-77-5
225116-01-8
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PEP (Properties); BIOL (Biological study); PROC (Process)
(increased lipophilicity and subsequent cell partitioning decrease passive transcellular diffusion of novel, highly lipophilic antioxidants)
RN 157012-18-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

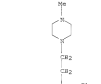


RN 157012-32-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-phenyl-7-[2-[1-piperazinyl]ethyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

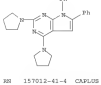


RN 157012-34-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(4-methyl-1-piperazinyl)ethyl]-6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

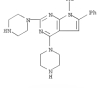


RN 157012-38-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-diphenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

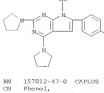
L5 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-41-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-phenyl-2,4-di-1-piperazinyl- (9CI) (CA INDEX NAME)

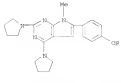


RN 157012-46-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

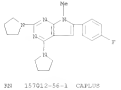


RN 157012-47-0 CAPLUS
CN Phenol, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)

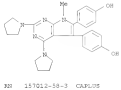
L5 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-48-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-fluorophenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

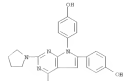


RN 157012-56-1 CAPLUS
CN Phenol, 4,4'-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidine-5,6-diyl)bis- (9CI) (CA INDEX NAME)

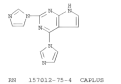


RN 157012-58-3 CAPLUS
CN Phenol, 4,4'-[2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidine-6,7-diyl]bis- (9CI) (CA INDEX NAME)

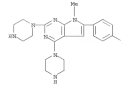
L5 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-61-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 2,4-di-1H-imidazol-1-yl- (9CI) (CA INDEX NAME)

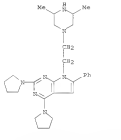


RN 157012-75-4 CAPLUS
CN Phenol, 4-(7-methyl-2,4-di-1-piperazinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)

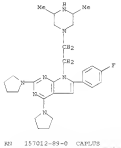


L5 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157012-84-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(3,5-dimethyl-1-piperazinyl)ethyl]-6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

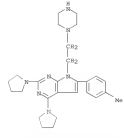


RN 157012-86-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-[4-(4-fluorophenyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

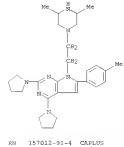


RN 157012-89-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-[4-methylphenyl]-7-[2-[1-piperazinyl]ethyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 20 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

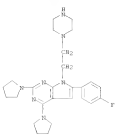


RN 157012-90-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(3,5-dimethyl-1-piperazinyl)ethyl]-6-[4-methylphenyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

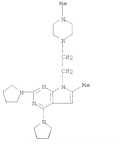


RN 157012-91-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-fluorophenyl)-7-[2-[1-piperazinyl]ethyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157013-79-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-methyl-7-[2-[4-methyl-1-piperazinyl]ethyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



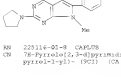
RN 157013-31-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-methyl-7-[2-(1-piperazinyl)ethyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157013-34-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

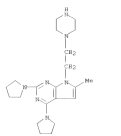
RN 225115-52-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(1,1-dimethylethyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 225115-77-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-(4-methylphenyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

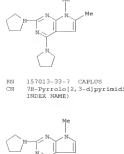


RN 225114-01-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-phenyl-2-(1-pyrrolidinyl)-4-(1H-pyrrol-1-yl)- (9CI) (CA INDEX NAME)

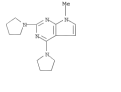
L5 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



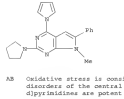
RN 157013-32-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



RN 157013-33-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



L5 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

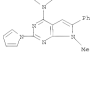


AB Oxidative stress is considered a cause or propagator of acute and chronic disorders of the central nervous system. Novel 2,4-diamino-pyrrolo[2,3-d]pyrimidines are potent inhibitors of iron-dependent lipid peroxidn., are cytoprotective in cell culture models of oxidative injury, and are neuroprotective in brain injury and ischemia models. The selection of lead candidates from this series required that they reach target cells deep within brain tissue in efficacious amts. after oral dosing. A homologous series of 26 highly lipophilic pyrrolopyrimidines was examined using cultured cell monolayers to understand the structure-permeability relationship and to use this information to predict brain penetration and residence time. Pyrrolopyrimidines were shown to be a more permeable structural class of membrane-interactive antioxidants where transepithelial permeability was inversely related to lipophilicity or to cell partitioning. Pyrrole substitutions influence cell partitioning where bulky hydrophobic groups increased partitioning and decreased permeability and smaller hydrophobic groups and more hydrophilic groups, especially those capable of weak hydrogen bonding, decreased partitioning, and increased permeability. Transmonolayer diffusion for these membrane-interactive antioxidants was limited mostly by desorption from the receiver-side membrane into the buffer. Thus, in this case, these in vitro cell monolayer models do not adequately mimic the in vivo situation by underestimating in vivo bioavailability of highly lipophilic compds. unless acceptors, such as serum proteins, are added to the receiving buffer.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 21 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:622209 CAPLUS
DOCUMENT NUMBER: 129:343459
TITLE: Chemical Oxidation of 2,4-Diaminopyrrolo[2,3-d]pyrimidines
AUTHOR(S): Rundy, Gordon L.; Gromhaw, Robert S.; Hazitt, Lee S.; Palmer, John R.; Mitsak, Stephen A.; Han, Fusen
CORPORATE SOURCE: Medicinal Chemistry and Structural Analytical and Medicinal Chemistry, Pharmacia Upjohn Company, Kalamazoo, MI, 49001-0199, USA
SOURCE: Journal of Organic Chemistry (1998), 63(21), 7542-7546
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:343459
IT 117012-10-7, PNU-87663
RL: RCT (Reactant; RACT (Reactant or reagent)
(oxidation of diaminopyrrolopyrimidines)
RN 117012-10-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

IT 215385-62-9P 215385-63-0P
RL: SYN (Synthetic preparation); PREP (Preparation)
(oxidation of diaminopyrrolopyrimidines)
RN 215385-62-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-phenyl-4-(1-pyrrolidinyl)-2-(1H-pyrrol-3-yl)- (9CI) (CA INDEX NAME)

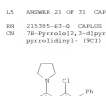


L5 ANSWER 22 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:780792 CAPLUS
DOCUMENT NUMBER: 128:304024
TITLE: Contribution of serum protein association to discrepancy between the in vivo and in vitro UDS results for 6,7-dimethyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidine (U-89843)
AUTHOR(S): Shaw, Ehipany, Koeplinger, Kenneth A.; Padbury, Guy E.; Aaron, Charles S.; Barbach, Philip R.; Mayo, Judy K.; Mattes, William B.; Rundy, Gordon L.
CORPORATE SOURCE: Drug Metabolism Research, Pharmacia and Upjohn Inc., Kalamazoo, MI, 49001, USA
SOURCE: Mutation Research, Genetic Toxicology and Environmental Mutagenesis (1997), 395(2,3), 119-126
CODEN: MGMTF3; ISSN: 1383-5718
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 117012-32-6, U 89843
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(contribution of serum protein association to discrepancy between in vivo
and in vitro UDS results for U-89843)
RN 117012-32-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

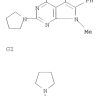
IT 174794-28-4, U 97924
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(contribution of serum protein association to discrepancy between in vivo
and in vitro UDS results for U-89843)
RN 174794-28-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-6-methanol, 7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 23 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 215385-63-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 5-chloro-7-methyl-6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

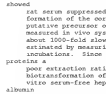


GI



AB Oxidation of lipophilic antioxidant PNU-87663 by a variety of nonbiol. oxidizing agents was investigated. E.g., stirring CHCl3 solns. of PNU-87663 in air for 1 wk gave small amts. of I and II. None of the oxidation products retained significant levels of lipid peroxidn. inhibiting activity.
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 22 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB U-89843 has been shown to undergo biotransformation, both in vitro and in vivo, to form U-97924 as a major primary metabolite. U-89843 was found to be pos. in an in vitro UDS mutagenesis screen conducted with primary rat hepatocytes in serum-free media. In contrast to in vitro results, no evidence of genetic toxicity of U-89843 was observed in rats in the in vivo/in vitro version of the UDS test with single oral doses up to 1400 mg/kg. The neg. results may be related to more robust in vivo detoxification mechanisms or relatively lower exposure to reactive metabolites formed by bioactivation of U-89843 as compared to that observed in the serum-free in vitro hepatocyte test system. Further studies showed rat serum suppressed the in vitro metabolism of U-89843 as well as the formation of the corresponding hydroxylated metabolite, U-97924, the putative precursor of proposed reactive electrophilic metabolite. The measured in vivo systemic clearance of U-89843 (0.53 l/h/kg) in rats was about 1000-fold slower than the in vitro intrinsic clearance (606 l/h/kg) estimated by measuring the formation of U-97924 in rat liver microsomal incubations. Since U-89843 is extensively associated with serum proteins a poor extraction ratio into the liver may account for the slower biotransformation of U-89843 in vivo as compared to that exhibited in in vitro serum-free hepatocyte incubations. Addition of bovine serum albumin (1-40 mg/mL) to the in vitro UDS assay medium decreased the UDS mean net grains per nucleus response of U-89843. These results suggest that the effect of serum protein should be considered when comparing serum-free in vitro UDS and in vivo UDS results for highly serum protein bound compds.
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 23 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:395768 CAPLUS
DOCUMENT NUMBER: 127:60535
TITLE: Effect of lazaroids U74389F and U89043D on iron-induced degeneration of nigrostriatal dopaminergic neurons
AUTHOR(S): Crandall, B. M.; Sengstock, G. J.; Arendash, G. W.
CORPORATE SOURCE: Department of Biology and Institute on Aging, University of South Florida, Tampa, FL, 33620, USA
SOURCE: Metal Ions in Biology and Medicine, Proceedings of the International Symposium on Metal Ions in Biology and Medicine, 4th, Barcelona, May 19-22, 1996 (1996), 317-319. Editor(s): Collery, Philippe. Libbey Eurotext: Montrouge, Fr.
CODEN: 64QOAC
DOCUMENT TYPE: Conference
LANGUAGE: English
IT 175297-45-7, U89043D
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(lazaroids U74389F and U89043D inhibition of iron-induced degeneration of nigrostriatal dopaminergic neurons)
RN 175297-45-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 157013-32-6
CMF C16 H23 N5

CM 2

CRN 7664-93-9
CMF H2 O4 S

L5 ANSWER 24 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:318586 CAPLUS
DOCUMENT NUMBER: 127:44777
TITLE: Pyrrolopyrimidines: novel brain-penetrating antioxidants with neuroprotective activity in brain injury and ischemia models
AUTHOR(S): Hall, E. D.; Andrus, P. K.; Smith, S. L.; Fleck, T. J.; Scherch, H. M.; Lutzke, B. S.; Sawada, G. A.; Althaus, J. S.; Vonvoigtlander, P. F.; Padbury, G. E.;
Larson, P. G.; Palmer, J. R.; Bundy, G. L.
CORPORATE SOURCE: CNS Diseases Research, Pharmacia Upjohn, Inc., Kalamazoo, MI, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (1997), 281(2), 895-904
CODEN: JPETAB, ISSN: 0022-3565
PUBLISHER: Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 172035-70-0, U 89663E 172035-71-1, U 89843E
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(pyrrolopyrimidines: brain-penetrating antioxidants with neuroprotective activity in brain injury and ischemia)
RN 172035-70-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-phenyl-2,4-di-1-pyrrolidinyl-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 157012-18-5
CMF C21 H23 N5

CM 2

CRN 75-75-2
CMF C H4 O3 S

L5 ANSWER 23 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB The substantia nigra zona compacta (SNc) of Parkinson's diseased (PD) brains shows a spontaneous increase in iron (Fe) concentration. Since Fe is known to facilitate reactions that result in free radical formation and oxidative damage, Fe may be a causative factor in the degeneration of nigrostriatal dopaminergic neurons that occurs in PD. Two lazaroid antioxidants - U74389F and U89043D - were tested for their ability to protect against the neurotoxic effects produced by Fe infusion into the rat SNc. U74389F treatment prevented acute increases in striatal dopamine and HVA levels normally present at 24 h following intranigral Fe infusion and attenuated the loss of SNc neurons normally present at 2 mo after intranigral Fe infusion. Chronic treatment with U89043D not only prevented Fe-induced atrophy of the SN at two weeks following Fe infusion, but also prevented the Fe-induced increase in the striatal dopamine turnover present at the same point.

L5 ANSWER 24 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 172035-71-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 157013-32-6
CMF C16 H23 N5

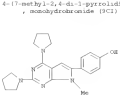
CM 2

CRN 75-75-2
CMF C H4 O3 S

AB A novel group of antioxidant compds., the pyrrolopyrimidines, has been discovered recently. Many of these possess significantly improved oral bioavailability (58-79% in rats), increased efficacy and potency in protecting cultured neurons against iron-induced lipid peroxidative injury and as much as a 5-fold increase in brain uptake compared with the 21-aminosteroid antioxidant compound, tirilazad mesylate (U-74006F), described earlier. They appear to quench lipid peroxidn. reactions by electron-donating and/or radical-trapping mechanisms. Several compds. in the series, such as U-101033E and U-104067F, demonstrate greater ability than tirilazad to protect the hippocampal CA1 region in the gerbil transient (5-min) forebrain ischemia model. Delaying treatment until 4 h after the ischemic insult still results in significant CA1 neuronal protection. U-101033E is still effective in salvaging a portion of the

L5 ANSWER 24 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CA1 neuronal pogelation when the ischemic duration is extended to 10 min. In addn., U-101033E has been found to be protective in the context of focal cerebral ischemia, reducing infarct size in the mouse permanent middle cerebral artery occlusion model, in contrast to tirilazad which is minimally effective. These results suggest that antioxidant compds. with improved brain parenchymal penetration are better able to limit certain types of ischemic brain damage than those which are localized in the cerebral microvasculature. However, the activity of U-101033E in improving early post-traumatic recovery in mice subjected to severe contusive head injury is similar to that of tirilazad. Last, the oral bioavailability of many pyrrolopyrimidines suggests that they may be useful for certain chronic neurodegenerative disorders in which lipid peroxidn. plays a role.
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

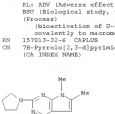
L5 ANSWER 25 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:745098 CAPLUS
DOCUMENT NUMBER: 126:15811
TITLE: Effects of lazaroids and a peroxynitrite scavenger in a cell model of peroxynitrite toxicity
AUTHOR(S): Fiel, Gregory J., Altaus, John S., VonVoigtlander, Philip F.
CORPORATE SOURCE: CNS Diseases Research, Pharmacia Upjohn Inc., Kalamazoo, MI, USA
SOURCE: Free Radical Biology & Medicine (1996), Volume Date 1997, 22(1/2), 223-228
CODEN: FRBMEL; ISSN: 0891-5849
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 172035-73-3, U 91726B
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(cytoprotection against peroxynitrite toxicity to cerebellar granular cells)
RN 172035-73-3 CAPLUS
CN Phenol, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

AB The authors developed a cerebellar granule cell model of peroxynitrite toxicity and showed that certain sulfhydryl-containing compds. (e.g., penicillamine) present as concurrent treatments ovoid inhibit this toxicity. In the present study, 21-aminosteroid and pyrrolopyrimidine lazaroids were tested for cytoprotection in this peroxynitrite toxicity model. In addition, the authors tested for added protection using a peroxynitrite scavenger concurrent treatment combined with a lazaroid post-treatment. The toxicity assay utilized cells that were previously exposed to 300 μM L-buthionine [S,R]-sulfoximine (BSO), an inhibitor of γ-glutamyl cysteine synthetase, for 24 h. This sublethal concentration of BSO shifted the peroxynitrite (3-1000 μM) toxicity curve to the left by more than one-half of a log unit. The half-maximal toxicity concentration (TC50)

L5 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:646457 CAPLUS
DOCUMENT NUMBER: 121:292176
TITLE: Bioactivation of 6,7-Dimethyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidine (U-89843) to Reactive Intermediates That Bind Covalently to Macromolecules and Produce Genotoxicity
AUTHOR(S): Ibao, Zhiyang; Koeplinger, Kenneth A.; Padbury, Guy E.; Bauer, Michael J.; Bundy, Gordon L.; Benatt, Lee S.; Schwartz, Theresa M.; Zimmermann, David C.; Harbach, Philip R.; et al.
CORPORATE SOURCE: Pharmacia Upjohn Inc., Kalamazoo, MI, 49001, USA
SOURCE: Chemical Research in Toxicology (1994), 7(8), 1230-1239
CODEN: CRTOEC; ISSN: 0893-228X
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 157013-32-6, U 89843
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(bioactivation of U-89843 to reactive intermediates that bind covalently to macromols. and produce genotoxicity)
RN 157013-32-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



IT 182146-03-8P, U 107634
RL: ADV (Adverse effect, including toxicity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(bioactivation of U-89843 to reactive intermediates that bind covalently to macromols. and produce genotoxicity)
RN 182146-03-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-ethyl-2,4-di-1-pyrrolidinyl-6-(trifluoroethyl)- (9CI) (CA INDEX NAME)

L5 ANSWER 27 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
of peroxynitrite in cells treated with BSO was 50 μM. The 21-aminosteroids, U-74006F and U-74500A, and the pyrrolopyrimidines, U-91768 and U-101033E, were tested as post-treatments. U-74006F and U-74500A had EC50 values of approx. 100 μM (concns. which blocked 50% of the toxicity). U-91768 and U-101033E had EC50 values of 3 μM and showed 100% protection at 3-10 μM. Treatment with either 100 μM U-74006F or 1 μM U-101033E resulted in a right-hand shift (protection) in the peroxynitrite toxicity curve. Combination treatment of lazaroids with 3 mM penicillamine resulted in additive protection compared to either treatment alone.

L5 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 174792-73-1, U 97985 174794-18-6, U 97924
182057-82-4 182057-84-6 182057-87-0
182057-90-5 182057-94-9
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(bioactivation of U-89843 to reactive intermediates that bind covalently to macromols. and produce genotoxicity)

RN 174792-73-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxaldehyde, 7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 174794-18-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-6-methanol, 7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 182057-81-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,6'-(oxybis(methylene))bis[7-methyl-2,4-di-1-

L5 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
pyrrolo[2,3-d]pyrimidin-6-yl)methyl]-L-cysteinyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 182057-94-9 CAPLUS
CN L-Cysteine, N-acetyl-S-[(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)methyl]- (9CI) (CA INDEX NAME)

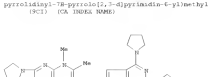
Absolute stereochemistry.

IT 182146-02-7, U 98140
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); SPN (Synthetic preparation); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation)
(bioactivation of U-89843 to reactive intermediates that bind covalently to macromols. and produce genotoxicity)

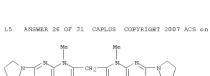
RN 182146-02-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,6'-methylenebis[7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 182057-84-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-5-[(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)methyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

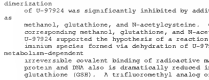


RN 182057-87-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(methoxymethyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



RN 182057-90-5 CAPLUS
CN Glycine, N-[N-L-γ-glutamyl-S-[(7-methyl-2,4-di-1-pyrrolidinyl-7H-

L5 ANSWER 26 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB U-89843 is a novel pyrrolo[2,3-d]pyrimidine antioxidant with prophylactic activity in animal models of lung inflammation. During preclin. safety evaluation, U-89843 was found to give a pos. response in the in vitro unscheduled DNA synthesis (UDS) assay, an assay which measures DNA repair following chemical-induced DNA damage in metabolically competent rat hepatocytes. Incubation of [14C]U-89843 with liver microsomes resulted in covalent binding of radioactive material to macromols. by a process that was NADPH-dependent. U-89843 has been shown to undergo C-6 methylhydroxylation to give U-97924, as rat both in vivo and in vitro, in a reaction catalyzed by cytochrome P 450 2C11. Synthetical U-97924 is chemical reactive and undergoes dimerization in aqueous solution The dimerization of U-97924 was significantly inhibited by addition of nucleophiles such as methanol, glutathione, and N-acetylcysteine. Characterization of the corresponding methanol, glutathione, and N-acetylcysteine adducts of U-97924 supported the hypothesis of a reactive pathway involving reactive iminium species formed via dehydration of U-97924. The metabolism-dependent irreversible covalent binding of radioactive material to liver microsomal protein and DNA also is dramatically reduced in the presence of reduced glutathione (GSH). A trifluoromethyl analog of U-89843 was prepared in an effort to block the corresponding metabolic hydroxylation pathway. This new compound (U-107634) was found to be negl. in the in vitro UDS assay, and its metabolic susceptibility toward hydroxylation at the C-6 Me group was eliminated. These observations suggest that the pos. in vitro UDS results of U-89843 are mediated by the bioactivation of U-89843, leading to reactive electrophilic intermediates derived from the (hydroxymethyl)pyrrole metabolite U-97924.

L5 ANSWER 27 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:137790 CAPLUS
DOCUMENT NUMBER: 124:250833
TITLE: Inhibition of Ca2+-pump ATPase and the Na+/K+-pump ATPase by iron-generated free radicals. Protection by 6,7-dimethyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidine sulfate (U-89843D), a potent, novel, antioxidant/free radical scavenger
AUTHOR(S): Kuhn, Troy T.; Burda, Thomas R.; Vincenzi, Frank F.
CORPORATE SOURCE: Dep. Pharmacology, Univ. Washington, Seattle, WA, 98195, USA
SOURCE: Biochemical Pharmacology (1996), 51(4), 471-6
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 175297-45-7, U 89843D
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
(Uses)
(inhibition of Ca2+-pump ATPase and the Na+/K+-pump ATPase by iron-generated free radicals and protection by U-89843D)
RN 175297-45-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl-, sulfate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 157013-32-6
CMF C16 H23 N5

CM 2

CRN 7664-93-9
CMF H2 O4 S

L5 ANSWER 28 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:174812 CAPLUS
DOCUMENT NUMBER: 124:229309
TITLE: In vitro and in vivo biotransformation of 6,7-dimethyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidine (U-89843) in the rat
AUTHOR(S): Zhao, Shuyang; Koeplinger, Kenneth A.; Bundy, Gordon L.; Bamitz, Lee E.; Padbury, Guy E.; Rawe, Michael J.; Sanders, Phillip E.
CORPORATE SOURCE: Drug Metabolism Research and Medicinal Chemistry Research, The Upjohn Company, Kalamazoo, MI, 49001, USA
SOURCE: Drug Metabolism and Disposition (1994), 22(2), 187-98
CODEN: DMDSAY; ISSN: 0090-9556
PUBLISHER: Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 157013-32-6, U 89843
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)
(biotransformation of pyrrolidinylpyrrolopyrimidine U-89843 in the rat)
RN 157013-32-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

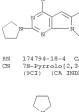
IT 174752-74-0 174752-75-1, U 89865 174794-28-4, U 97924
RL: BSU (Biological study, unclassified); MTH (Metabolic formation); BIOL (Biological study); FORM (Formation, nonpreparative)
(biotransformation of pyrrolidinylpyrrolopyrimidine U-89843 in the rat)
RN 174752-74-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxylic acid, 7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 27 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB Preincubation of red blood cell (RBC) membranes with a model system known to generate reactive oxygen species (ROS) and free radicals (200 μM ferrous sulfate and 200 μM EDTA, Fe2+/EDTA) resulted in inhibition of the Na+/K+-pump ATPase, the basal Ca2+-pump ATPase, and the calmodulin-activated Ca2+-pump ATPase. Inhibition of the ion pump ATPases
was also associated with membrane protein crosslinking and lipid peroxidn., the latter as monitored by the formation of thiobarbituric acid reactive substances (TBARS). Inhibition of the ion transport ATPases, protein crosslinking and formation of TBARS were prevented by U-89843D in a concentration-dependent manner, with half-maximal protection seen at 0.3 μM.
U-89843D was more potent than the classical antioxidant butylated hydroxytoluene. Neither U-89843D nor the solvent DMSO had any effect on the assay of TBARS. U-89843D exerted only minimal inhibitory activity on ATPase activities. Thus, U-89843D was potent in vitro in preventing a variety of membrane-damaging reactions mediated by ROS. It is suggested that protection of membranes from ROS-mediated damage is of potential usefulness in the prevention and treatment of certain disease processes.

L5 ANSWER 28 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 174752-75-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-6-carboxaldehyde, 7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



RN 174794-28-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-6-methanol, 7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

AB The biotransformation of 6,7-dimethyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidine (U-89843) has been studied in rat both in vitro and in vivo. Major metabolites observed by HPLC anal. of rat plasma, liver cytosol, and
microsomal incubations were characterized by UV, LC/MS, and comparison with synthetic stds. The structures of the metabolites were shown to be the C-6 hydroxymethyl (U-97924), C-6 formyl (U-97865), and C-6 carboxyl analogs of U-89843. In the male rat, formation of U-97924 is mediated by cytochrome P 450(2c11. Kinetic anal. of U-97924 formation indicated that it was a high-affinity/high-capacity processs (KM = 4.2 ± 0.5 μM; Vmax = 21.2 ± 0.8 nmol/mg/min). Formation of U-97865 via enzymic oxidation from the primary metabolite U-97924 was catalyzed by both the microsomal subcellular fraction in a NADPH-dependent process (presumably

L5 ANSWER 28 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
via cytochrome P 450) and in cytosol by NAD+-dependent alc. dehydrogenase.
Upon incubation with cytosolic fractions, U-97865 was found to undergo NAd+-dependent oxidn., mediated by aldehyde dehydrogenase, to the corresponding carboxylic acid. Although significant levels of U-89843, U-97524, and U-97865 obsd. in vivo in rat plasma, only a minor amt. of the carboxylic acid together with larger amts. of unidentified polar metabolites were excreted in urine and feces.

L5 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:18990 CAPLUS
DOCUMENT NUMBER: 124:135448
TITLE: U-89843A is a novel allosteric modulator of γ-aminobutyric acidA receptors
AUTHOR(S): Im, Hansook K.; Im, Wha Bin; Pregenzer, Jeff F.; Carter, Don B.; Hamilton, Beverly J.
CORPORATE SOURCE: Central Nervous System Diseases Research, The Upjohn Company, Kalamazoo, MI, USA
SOURCE: Journal of Pharmacology and Experimental Therapeutics (1995), 275(3), 1392-5
CODEN: JPETAB; ISSN: 0022-3565
PUBLISHER: Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 157013-32-6, U 89843A
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(U-89843A is a novel allosteric modulator of γ-aminobutyric acidA receptors)
RN 157013-32-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 4,7-dimethyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

IT 157012-69-6, U 94047 157013-34-8, U 92229
157013-36-0, U 89640
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(sedation by pyrrolopyrimidines in relation to GABAA receptor modulation)
RN 157012-69-6 CAPLUS
CN Phenol, 2-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)

L5 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Benzodiazepine antagonist, was also obsd. in the α1β2γ2 and α6β2γ2 subtypes (no selectivity to different α-isoforms unlike many benzodiazepines), but was absent in the receptor subtypes consisting of two subunits (α1β2, α1γ2 and β2γ2). It has been known that neurosteroids and barbiturates are uniformly active in both the two subunit receptors, substituted pyrazolones are only active in the α1β2 subtype and loreclezole is active in the subtypes contg. β3. The authors propose that U-89843A interacts with an allosteric site on GABAA receptors distinct from the sites for benzodiazepines, barbiturates, neurosteroids, substituted pyrazolones or loreclezole. In the mouse, several analogs of U-89843A induced sedation with a rank order of potency identical to that obsd. for their actions on [35S]t-butylbicyclophosphorothionate binding and GABA-induced Cl- currents. Moreover, sedation induced by the analogs was not accompanied by a loss of righting reflex, unlike diazepam, barbiturates and neurosteroids. U-89843A appears to represent a novel class of allosteric modulators of GABAA receptors (pyrrolopyrimidines) and may possess a unique therapeutic profile, arising from its interaction with GABAA receptors via a novel site which is formed from quaternary assocns. of the α, β and γ subunits.

L5 ANSWER 29 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157013-34-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 157013-36-0 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 6-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

AB A group of pyrrolopyrimidine deriv. were examined for their interaction with rat recombinant γ-aminobutyric acid (GABA)A receptors using the whole cell patch clamp and equilibrium binding techniques. In the α1β2γ2 subtype of GABAA receptors expressed in human embryonic kidney cells, a prototype pyrrolopyrimidine, U-89843A [7H-pyrrolo[2,3-d]pyrimidine, 6,7-methyl-2,4-di-1-pyrrolidinyl, hydrochloride], dose-dependently enhanced 5 μM GABA-induced Cl- currents with a maximal enhancement of 2629, a half-maximal concentration of 2 μM and a slope factor of 1.1. The drug also inhibited [35S]t-butylbicyclophosphorothionate binding in rat cerebrocortical membranes with a similar half-maximal inhibitory concentration. The enhancement of Cl- currents by U-89843A was insensitive to Ro 15-1788 (a

L5 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:926911 CAPLUS
DOCUMENT NUMBER: 124:55909
TITLE: Synthesis of Novel 2,4-Diaminopyrrolo[2,3-d]pyrimidines with Antioxidant, Neuroprotective, and Antiastrea Activity
AUTHOR(S): Rundy, Gordon L.; Ayer, Donald E.; Barnett, Lee S.; Belonga, Kenneth L.; Misrak, Stephen A.; Palmer, John R.; Tustin, James M.; Chin, Jia En; Hall, Edward D.; et al.
CORPORATE SOURCE: Upjohn Laboratories, Upjohn Company, Kalamazoo, MI, 49001, USA
SOURCE: Journal of Medicinal Chemistry (1995), 38(21), 4161-3
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 124:55909
IT 157012-28-9P, U 87623 157012-46-9P, U 89623
157012-47-0P, U 91743 157013-32-6P, U 89843
172035-70-0P, U 87638 172035-71-1P, U 89843E
172035-72-2P, U 89623E 172035-73-3P, U 91743E
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of pyrrolo[2,3-d]pyrimidinediamines as antioxidants, neuroprotectants and antiasthmatics)
RN 157012-28-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-4-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 157012-46-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 4-(4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157012-47-0 CAPLUS
CN Phenol, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)

RN 157013-32-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 172035-70-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-phenyl-2,4-di-1-pyrrolidinyl-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

L5 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CRN 157012-28-9
CMF C21 H25 N5

CM 2

CRN 75-75-2
CMF C H4 O3 S

RN 172035-71-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 157013-32-6
CMF C16 H23 N5

CM 2

CRN 75-75-2
CMF C H4 O3 S

L5 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 172035-72-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 4-(4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

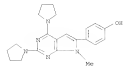
CRN 157012-46-9
CMF C22 H27 N5 O

CM 2

CRN 75-75-2
CMF C H4 O3 S

RN 172035-73-3 CAPLUS
CN Phenol, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

L5 ANSWER 30 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HBr

AB Several novel 2,4-diaminopyrrolo[2,3-d]pyrimidines were prepared from 2,4,6-triaminopyrimidines and a-bromo ketones under mildly basic conditions. Many of these compds. are potent inhibitors of iron-dependent lipid peroxidn., they exhibit cytoprotective activity in two cell culture models of oxidative injury, and they possess neuroprotective activity in a mouse head injury model. In addition, U-101033 [i.e., 5,6,7,8-tetrahydro-9-[2-(4-morpholinyl)ethyl]-2,4-di-1-pyrrolidinyl-1H-pyrimido[4,5-b]indole] and U-104067 [i.e., 9-[2-(4-morpholinyl)ethyl]-2,4-di-1-pyrrolidinyl-1H-pyrimido[4,5-b]indole] are both effective inhibitors of antigen-induced lung eosinophilia in mice and rats (anti-asthma model) with potencies close to the glucocorticoids. Compound U-104067 was selected for clin. evaluation for the treatment of asthma and several chronic neurodegenerative disorders.

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:534139 CAPLUS
DOCUMENT NUMBER: 121:134139
TITLE: Preparation of pharmaceutically active bicyclic-heterocyclic amines
INVENTOR(S): Ayer, Donald E.; Bundy, Gordon L.; Jacobsen, Eric Jon
PATENT ASSIGNEE(S): Upjohn Co., USA
SOURCE: PCT Int. Appl., 120 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9320078	A1	19931014	WO 1993-US2188	19930316
W: AT, AU, BB, BG, BR, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9339174	A	19931108	AU 1993-39174	19930316
AU 675932	B2	19970227		
EP 633886	A1	19950118	EP 1993-908303	19930316
EP 633886	B1	20001018		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
HU 70954	A2	19951128	HU 1994-2829	19930316
JP 08502721	T	19960326	JP 1993-517457	19930316
RU 2103272	C1	19980127	RU 1994-42466	19930316
PL 175347	B1	19981231	PL 1993-305430	19930316
PL 175327	B1	19981231	PL 1993-317810	19930316
AT 197051	T	20001115	AT 1993-908303	19930316
ES 2150941	T3	20001216	ES 1993-908303	19930316
PT 633886	T	20010330	PT 1993-908303	19930316
NO 9403655	A	19941205	NO 1994-3655	19940930
NO 303542	B1	19980727		
FI 9404602	A	19941003	FI 1994-4602	19941003
US 5502187	A	19960326	US 1994-317934	19941003
GR 3035188	T3	20010430	GR 2001-400006	20010104
LV 12794	B	20020620	LV 2001-150	20011018
PRIORITY APPLN. INFO.:			US 1992-863646	A2 19920403
			WO 1993-US2188	A 19930316
			US 1993-128957	B1 19930929
			US 1994-222995	B1 19940405

OTHER SOURCE(S): CASREACT 121:134139; MARPAT 121:134139

IT 157012-18-5P 157012-19-6P 157012-21-0P
157012-22-1P 157012-23-2P 157012-24-3P
157012-25-4P 157012-26-5P 157012-27-6P
157012-28-7P 157012-29-8P 157012-30-1P

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

157012-31-2P 157012-32-3P 157012-33-4P
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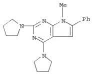
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

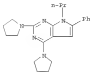
157014-12-5P 157014-13-6P 157014-14-7P
157014-49-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as drug)

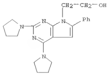
RN 157012-18-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



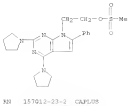
RN 157012-19-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-phenyl-7-propyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



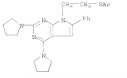
RN 157012-21-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanol, 6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



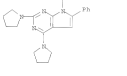
L5 ANSWER 31 OF 33 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 157012-22-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanol, 4-phenyl-2,4-di-1-pyrrolidinyl-, methanesulfonate (ester) (9CI) (CA INDEX NAME)



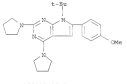
RN 157012-23-2 CAPLUS
CN Ethanethioic acid, S-[2-(4-phenyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-7-yl)ethyl] ester (9CI) (CA INDEX NAME)



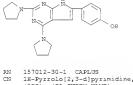
RN 157012-24-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanethiol, 4-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



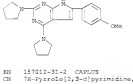
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-29-8 CAPLUS
CN Phenol, 4-(2,4-di-1-pyrrolidinyl-1H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)

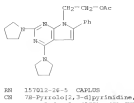


RN 157012-30-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 6-(4-methoxyphenyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

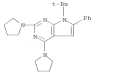


RN 157012-31-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-4-phenyl-2,4-di-4-thiomorpholinyl- (9CI) (CA INDEX NAME)

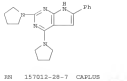
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 157012-25-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanol, 4-phenyl-2,4-di-1-pyrrolidinyl-, acetate (ester) (9CI) (CA INDEX NAME)



RN 157012-26-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[1,1-dimethylethyl)-6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

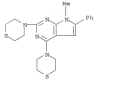


RN 157012-27-6 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

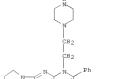


RN 157012-28-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-(1,1-dimethylethyl)-6-(4-methoxyphenyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

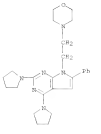


RN 157012-32-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-phenyl-7-[2-(1-piperazinyl)ethyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

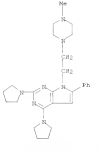


RN 157012-33-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(4-morpholinyl)ethyl]-6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

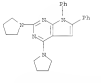


RN 157012-34-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(4-methyl-1-piperazinyl)ethyl]-6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

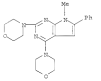


RN 157012-35-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanol, 6-(4-methoxyphenyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

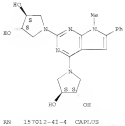


RN 157012-39-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-2,4-di-4-morpholinyl-6-phenyl- (9CI) (CA INDEX NAME)



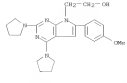
RN 157012-40-3 CAPLUS
CN 3,4-Pyrrolidinediol, 2,2'-[7-methyl-6-phenyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diyl]bis-, [3R-[1(3*,4*),2a,4β]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

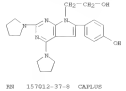


RN 157012-41-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-phenyl-2,4-di-1-piperazinyl- (9CI)

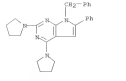
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-36-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanol, 6-(4-hydroxyphenyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

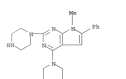


RN 157012-37-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-phenyl-7-(phenylmethyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



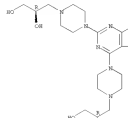
RN 157012-38-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-diphenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued) (CA INDEX NAME)



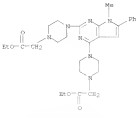
RN 157012-42-5 CAPLUS
CN 1,2-Propanediol, 3,3'-[[7-methyl-6-phenyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diyl]di-4,1-piperazinediyl]bis-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

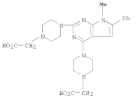


RN 157012-43-6 CAPLUS
CN 1-Piperazineacetic acid, 4,4'-(7-methyl-6-phenyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diyl)bis-, diethyl ester (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

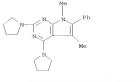


RN 157012-44-7 CAPLUS
CN 1-Piperazineacetic acid, 4,4'-(7-methyl-6-phenyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diyl)bis- (9CI) (CA INDEX NAME)

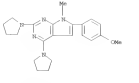


RN 157012-43-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 5,7-dimethyl-6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

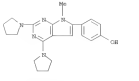
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-46-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

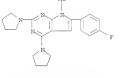


RN 157012-47-0 CAPLUS
CN Phenol, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)

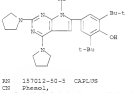


RN 157012-48-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-fluorophenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

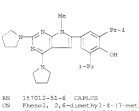
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-49-2 CAPLUS
CN Phenol, 2,6-bis[1,1-dimethylethyl)-4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)

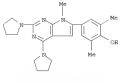


RN 157012-50-5 CAPLUS
CN Phenol, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-2,6-bis[1-methylethyl)- (9CI) (CA INDEX NAME)

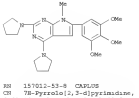


RN 157012-51-6 CAPLUS
CN Phenol, 2,6-diethyl-4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)

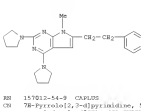
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-52-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-2,4-di-1-pyrrolidinyl-6-[3,4,5-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

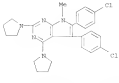


RN 157012-53-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-[2-[4-methoxyphenyl]ethyl]-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

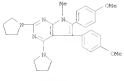


RN 157012-54-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 5,6-bis(4-chlorophenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

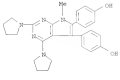
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-59-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 5,6-bis(4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

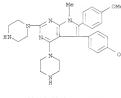


RN 157012-58-1 CAPLUS
CN Phenol, 4,4'-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidine-5,6-diyl)bis- (9CI) (CA INDEX NAME)

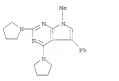


RN 157012-57-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-bis(4-methoxyphenyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

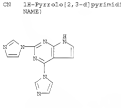
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-60-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-5-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

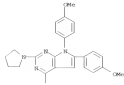


RN 157012-61-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 2,4-di-1H-imidazol-1-yl- (9CI) (CA INDEX NAME)

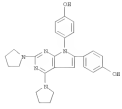


RN 157012-62-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanesulfonic acid, 4-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

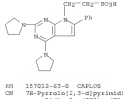


RN 157012-58-3 CAPLUS
CN Phenol, 4,4'-(2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidine-6,7-diyl)bis- (9CI) (CA INDEX NAME)

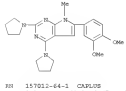


RN 157012-59-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 5,6-bis(4-methoxyphenyl)-7-methyl-2,4-di-1-piperazinyl- (9CI) (CA INDEX NAME)

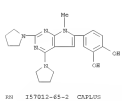
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-63-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(3,4-dimethoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

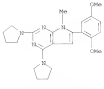


RN 157012-64-1 CAPLUS
CN 1,2-Benzenediol, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)

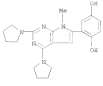


RN 157012-65-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(2,5-dimethoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

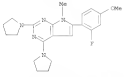
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-66-3 CAPLUS
CN 2,4-Benzenediol, 2-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)

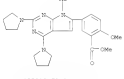


RN 157012-67-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(2-fluoro-4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

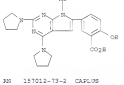


RN 157012-68-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(2-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

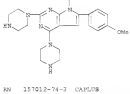
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-72-3 CAPLUS
CN Benzoic acid, 2-hydroxy-3-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)



RN 157012-73-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-methoxyphenyl)-7-methyl-2,4-di-1-piperazinyl- (9CI) (CA INDEX NAME)

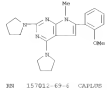


RN 157012-74-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-methoxyphenyl)-7-methyl-2,4-di-1-piperazinyl-, dimethanesulfonate (9CI) (CA INDEX NAME)

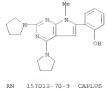
CM 1

CRN 157012-73-2
CMF C22 H29 N7 O

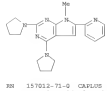
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-69-6 CAPLUS
CN Phenol, 2-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)

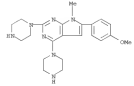


RN 157012-70-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-(2-pyridinyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



RN 157012-71-0 CAPLUS
CN Benzoic acid, 2-methoxy-5-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, methyl ester (9CI) (CA INDEX NAME)

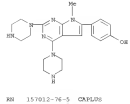
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

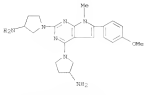
CRN 75-75-2
CMF C H4 O3 S

RN 157012-75-4 CAPLUS
CN Phenol, 4-(7-methyl-2,4-di-1-piperazinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)- (9CI) (CA INDEX NAME)

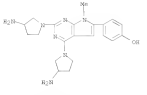


RN 157012-76-5 CAPLUS
CN 3-Pyrrolidinamine, 1,1'-[6-(4-methoxyphenyl)-7-methyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diyl]bis- (9CI) (CA INDEX NAME)

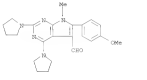
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-77-6 CAPLUS
CN Phenol, 4-[2,6-bis[3-amino-1-pyrrolidinyl]-7-methyl-7H-pyrrolo[2,3-d]pyrimidin-4-yl]- (9CI) (CA INDEX NAME)

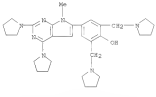


RN 157012-78-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxaldehyde, 6-(4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

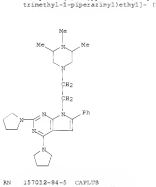


RN 157012-79-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-methanol, 6-(4-methoxyphenyl)-7-methyl-2,4-

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

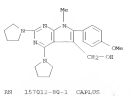


RN 157012-83-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-phenyl-2,4-di-1-pyrrolidinyl-7-[2-(3,4,5-trimethyl-1-piperazinyl)ethyl]- (9CI) (CA INDEX NAME)

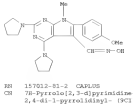


RN 157012-84-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(3,5-dimethyl-1-piperazinyl)ethyl]-6-phenyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

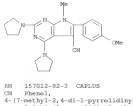
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



RN 157012-80-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carboxaldehyde, 6-(4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl-, oxime (9CI) (CA INDEX NAME)

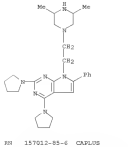


RN 157012-81-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-5-carbonitrile, 6-(4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

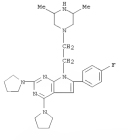


RN 157012-82-3 CAPLUS
CN Phenol, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-2,6-bis[1-pyrrolidinylmethyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

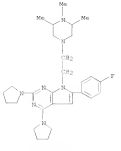


RN 157012-85-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(3,5-dimethyl-1-piperazinyl)ethyl]-6-[4-fluorophenyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

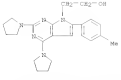


RN 157012-86-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-fluorophenyl)-2,4-di-1-pyrrolidinyl-7-[2-(3,4,5-trimethyl-1-piperazinyl)ethyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

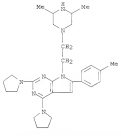


RN 157012-87-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanol, 6-(4-methylphenyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

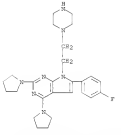


RN 157012-88-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-methylphenyl)-2,4-di-1-pyrrolidinyl-7-[2-(3,4,5-trimethyl-1-piperazinyl)ethyl]- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

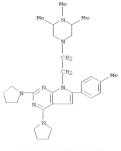


RN 157012-91-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-fluorophenyl)-7-[2-[1-piperazinyl)ethyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

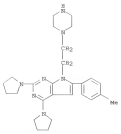


RN 157012-92-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 5-methyl-6-(4-methylphenyl)-7-[2-(1-piperazinyl)ethyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

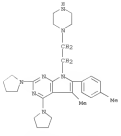


RN 157012-89-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-methylphenyl)-7-[2-(1-piperazinyl)ethyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

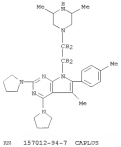


RN 157012-90-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(3,5-dimethyl-1-piperazinyl)ethyl]-6-(4-methylphenyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

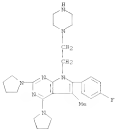


RN 157012-93-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(3,5-dumethyl-1-piperazinyl)ethyl]-5-methyl-6-(4-methylphenyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

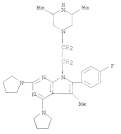


RN 157012-94-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-fluorophenyl)-5-methyl-7-[2-(1-piperazinyl)ethyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

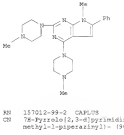


RN 157012-95-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(3,5-dimethyl-1-piperazinyl)ethyl]-6-(4-fluorophenyl)-3-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

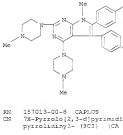


RN 157012-96-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-methoxyphenyl)-7-methyl-2,4-bis(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

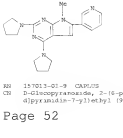
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157012-99-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 5,6-bis(4-methoxyphenyl)-7-methyl-2,4-bis(4-methyl-1-piperazinyl)- (9CI) (CA INDEX NAME)

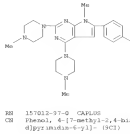


RN 157013-02-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-(3-pyridinyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

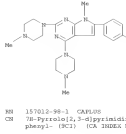


RN 157013-07-9 CAPLUS
CN D-Glucopyranoside, 2-(6-phenyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-7-yl)ethyl (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



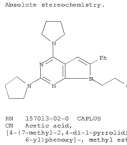
RN 157012-97-0 CAPLUS
CN Phenol, 4-[7-methyl-2,4-bis(4-methyl-1-piperazinyl)-7H-pyrrolo[2,3-d]pyrimidin-6-yl]- (9CI) (CA INDEX NAME)



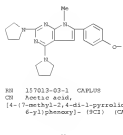
RN 157012-98-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-2,4-bis(4-methyl-1-piperazinyl)-6-phenyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

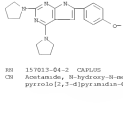
Absolute stereochemistry.



RN 157013-02-0 CAPLUS
CN Acetic acid, [4-[7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl]phenoxy]-, methyl ester (9CI) (CA INDEX NAME)

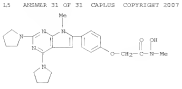


RN 157013-03-1 CAPLUS
CN Acetic acid, [4-[7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl]phenoxy]- (9CI) (CA INDEX NAME)

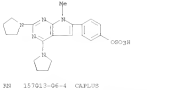


RN 157013-04-2 CAPLUS
CN Acetamide, N-hydroxy-N-methyl-2-[4-[7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl]phenoxy]- (9CI) (CA INDEX NAME)

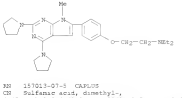
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157013-05-3 CAPLUS
CN Fbrzol,
4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-
, hydrogen sulfate (ester) (9CI) (CA INDEX NAME)

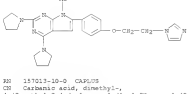


RN 157013-06-4 CAPLUS
CN Ethanamine, N,N-diethyl-2-[4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-
pyrrolo[2,3-d]pyrimidin-6-yl)phenoxy]- (9CI) (CA INDEX NAME)

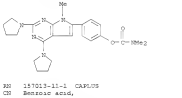


RN 157013-07-5 CAPLUS
CN Sulfamic acid, dimethyl-,
4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-
d]pyrimidin-6-yl)phenyl ester (9CI) (CA INDEX NAME)

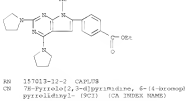
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157013-10-0 CAPLUS
CN Carbamic acid, dimethyl-,
4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-
d]pyrimidin-6-yl)phenyl ester (9CI) (CA INDEX NAME)

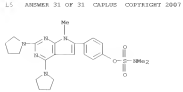


RN 157013-11-1 CAPLUS
CN Benzoic acid,
4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-
6-yl-, ethyl ester (9CI) (CA INDEX NAME)



RN 157013-12-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-bromophenyl)-7-methyl-2,4-di-1-
pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157013-08-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine,
6-[4-[2-[2-(2-methoxyethoxy)ethoxy]ph+
ny1]-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

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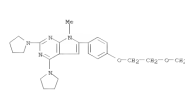

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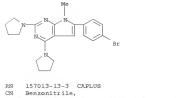
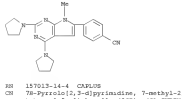
RN 157013-09-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-[4-[2-(1H-imidazol-1-ylethoxy)phenyl]-7-
methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

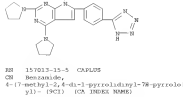
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157013-13-3 CAPLUS
CN Benzonitrile,
4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-
6-yl)- (9CI) (CA INDEX NAME)

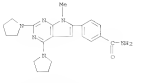


RN 157013-14-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-2,4-di-1-pyrrolidinyl-6-[4-(1H-
tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)

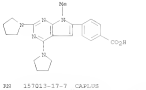


RN 157013-15-5 CAPLUS
CN Benzamide,
4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-
yl)- (9CI) (CA INDEX NAME)

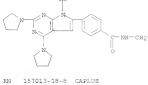
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157013-16-6 CAPLUS
CN Benzoic acid,
4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-
6-yl)- (9CI) (CA INDEX NAME)

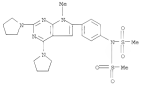


RN 157013-17-7 CAPLUS
CN Ethanesulfonic acid,
2-[(4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-
d]pyrimidin-6-yl)benzoyl]amino]- (9CI) (CA INDEX NAME)

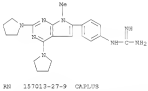


RN 157013-18-8 CAPLUS
CN Benzamide,
4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-
yl)-N-1H-tetrazol-5-yl- (9CI) (CA INDEX NAME)

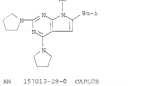
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157013-22-4 CAPLUS
CN Guanidine,
[4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-
yl)phenyl]- (9CI) (CA INDEX NAME)

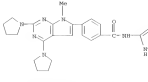


RN 157013-27-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-(2-methylpropyl)-2,4-di-1-
pyrrolidinyl- (9CI) (CA INDEX NAME)

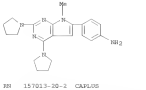


RN 157013-28-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanol, 6-methyl-2,4-di-1-pyrrolidinyl-
(9CI) (CA INDEX NAME)

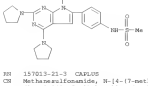
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157013-19-9 CAPLUS
CN Benzenamine,
4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-
6-yl)- (9CI) (CA INDEX NAME)

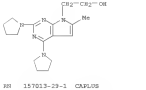


RN 157013-20-2 CAPLUS
CN Methanesulfonamide, N-[4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-
d]pyrimidin-6-yl)phenyl]- (9CI) (CA INDEX NAME)

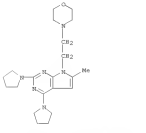


RN 157013-21-3 CAPLUS
CN Methanesulfonamide, N-[4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-
d]pyrimidin-6-yl)phenyl]-N-(methylsulfonyl)- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

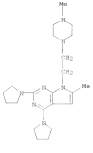


RN 157013-23-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine,
6-methyl-7-[2-[4-morpholinyl]ethyl]-2,4-di-1-
pyrrolidinyl- (9CI) (CA INDEX NAME)

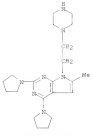


RN 157013-30-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine,
6-methyl-7-[2-[4-methyl-1-piperazinyl)ethyl]-
2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157013-31-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 4-methyl-7-[2-[1-(1-piperazinyl)ethyl]-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



RN 157013-32-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157013-37-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 4-methyl-2,4-di-1-pyrrolidinyl-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 157013-36-0
CMF C15 H21 N5

CM 2

CRN 76-05-1
CMF C2 H F3 O2

RN 157013-38-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-ethyl-4-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157013-33-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 157013-34-8 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 157013-35-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-ethyl-6-(1-methylethyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

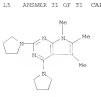
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157013-39-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-ethyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

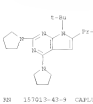
RN 157013-40-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-(1,1-dimethylethyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

RN 157013-41-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 5,6,7-trimethyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

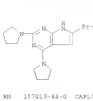
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157013-42-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-(1,1-dimethylethyl)-6-(1-methylethyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

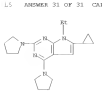


RN 157013-43-9 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 6-(1-methylethyl)-2,4-di-1-pyrrolidinyl-, monohydrochloride (9CI) (CA INDEX NAME)

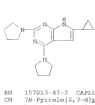


RN 157013-44-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-cyclopropyl-7-ethyl-2,4-di-1-pyrrolidinyl-, monohydrochloride (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157013-45-1 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 6-cyclopropyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)



RN 157013-47-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanol, 6-phenyl-2,4-di-1-pyrrolidinyl-, hydrochloride (9CI) (CA INDEX NAME)

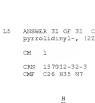
● x HCl

RN 157013-48-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-phenyl-7-[2-[1-piperazinyl]ethyl]-2,4-di-1-

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
pyrrolidinyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 157012-32-3
CMF C26 H35 N7



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

RN 157013-49-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-[4-morpholinyl]ethyl]-6-phenyl-2,4-di-1-pyrrolidinyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 157012-33-4
CMF C26 H34 N6 O

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 2

CRN 110-16-7
CMF C4 H4 O4

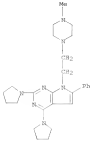
Double bond geometry as shown.

RN 157013-50-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-[4-ethyl-1-piperazinyl]ethyl]-6-phenyl-2,4-di-1-pyrrolidinyl-, (2Z)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 157012-34-5
CMF C27 H37 N7

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



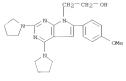
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

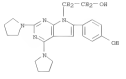
RN 157013-51-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanol, 6-[4-methoxyphenyl)-2,4-di-1-pyrrolidinyl-, hydrochloride (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● x HCl

RN 157013-52-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanol, 6-[4-hydroxyphenyl)-2,4-di-1-pyrrolidinyl-, hydrochloride (9CI) (CA INDEX NAME)



● x HCl

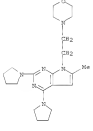
RN 157013-53-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine-7-ethanol, 6-methyl-2,4-di-1-pyrrolidinyl-, methanesulfonate (ester) (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157013-54-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine,
6-methyl-7-[2-[4-morpholinyl)ethyl]-2,4-di-1-pyrrolidinyl-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 157013-29-1
CMF C21 H32 N6 O



CM 2

CRN 110-16-7
CMF C4 H4 O4

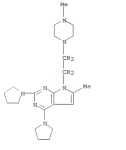
Double bond geometry as shown.

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157013-55-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine,
6-methyl-7-[2-[4-methyl-1-piperazinyl)ethyl]-2,4-di-1-pyrrolidinyl-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 157013-30-4
CMF C22 H35 N7



CM 2

CRN 110-16-7
CMF C4 H4 O4

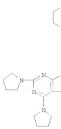
Double bond geometry as shown.

RN 157013-56-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine,
6-methyl-7-[2-[1-piperazinyl)ethyl]-2,4-di-1-pyrrolidinyl-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 157013-33-5
CMF C21 H33 N7



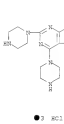
CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

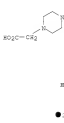
RN 157013-57-5 CAPLUS
CN Ethanone, 1-phenyl-2-(6-phenyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-7-yl)- (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● 3 HCl

RN 157013-60-0 CAPLUS
CN 1-Piperazineacetic acid, 4,4'-(7-methyl-6-phenyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diyl)bis-, dipotassium salt (9CI) (CA INDEX NAME)



● 2 K

RN 157013-61-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl-, methanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 157012-46-9
CMF C22 H27 N5 O

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157013-58-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-phenyl-2,4-di-1-pyrrolidinyl-, methanesulfonate (9CI) (CA INDEX NAME)

CM 1

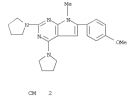
CRN 157012-18-5
CMF C21 H25 N5

CM 2

CRN 75-75-2
CMF C H4 O3 S

RN 157013-59-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-6-phenyl-2,4-di-1-piperazinyl-, trihydrochloride (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 75-75-2
CMF C H4 O3 S

RN 157013-62-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl-, methanesulfonate (9CI) (CA INDEX NAME)

CM 1

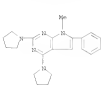
CRN 157013-32-4
CMF C16 H23 N5

CM 2

CRN 75-75-2
CMF C H4 O3 S

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157013-62-3 CAPLUS
CN Phenol,
4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-
, hydrobromide (9CI) (CA INDEX NAME)

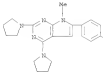


● x HBr

RN 157013-64-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-fluorophenyl)-7-methyl-2,4-di-1-pyrrolidinyl-, methanesulfonate (9CI) (CA INDEX NAME)

CM 1

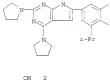
CRN 157012-48-1
CMF C21 H24 F N5



L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
NAME)

CM 1

CRN 157012-50-5
CMF C27 H37 N5 O



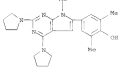
CM 2

CRN 75-75-2
CMF C H4 O3 S

RN 157013-67-7 CAPLUS
CN Phenol, 2,6-dimethyl-4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 157012-52-6
CMF C23 H29 N5 O



CM 2

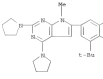
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CM 2

CRN 75-75-2
CMF C H4 O3 S

RN 157013-65-5 CAPLUS
CN Phenol, 2,6-bis(1,1-dimethylethyl)-4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, monomethanesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 157012-49-2
CMF C29 H41 N5 O



CM 2

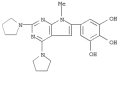
CRN 75-75-2
CMF C H4 O3 S

RN 157013-66-6 CAPLUS
CN Phenol,
4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-
2,6-bis(1-methylethyl)-, monomethanesulfonate (salt) (9CI) (CA INDEX

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CRN 75-75-2
CMF C H4 O3 S

RN 157013-68-8 CAPLUS
CN 1,2,3-Benzenetriol, 5-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, monohydrobromide (9CI) (CA INDEX NAME)

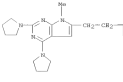


● HBr

RN 157012-69-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine,
6-[2-(4-methoxyphenyl)ethyl]-7-methyl-2,4-di-1-pyrrolidinyl-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

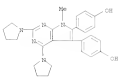
CRN 157012-53-8
CMF C24 H31 N5 O



L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CM 2

CRN 75-75-2
CMF C H4 O3 S

RN 157013-70-2 CAPLUS
CN Phenol, 4,4'-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidine-5,6-diyl)bis-, monohydrobromide (9CI) (CA INDEX NAME)



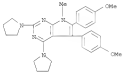
● HBr

RN 157013-71-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 5,6-bis(4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 157012-55-0
CMF C29 H33 N5 O2

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CRN 157012-55-0
CMF C29 H33 N5 O2



CM 2

CRN 75-75-2
CMF C H4 O3 S

RN 157013-74-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 2,4-di-1-pyrrolidinyl-, monomethanesulfonate (9CI) (CA INDEX NAME)

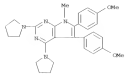
CM 1

CRN 157013-34-8
CMF C14 H19 N5

CM 2

CRN 75-75-2
CMF C H4 O3 S

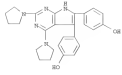
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 75-75-2
CMF C H4 O3 S

RN 157013-72-4 CAPLUS
CN Phenol, 4,4'-(2,4-di-1-pyrrolidinyl-1H-pyrrolo[2,3-d]pyrimidine-5,6-diyl)bis-, hydrobromide (9CI) (CA INDEX NAME)



● x HBr

RN 157013-73-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 5,6-bis(4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl-, dimethanesulfonate (9CI) (CA INDEX NAME)

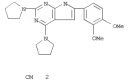
CM 1

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157013-75-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(3,4-dimethoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl-, monomethanesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 157012-63-0
CMF C23 H29 N5 O2

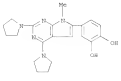


CM 2

CRN 75-75-2
CMF C H4 O3 S

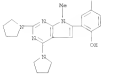
RN 157013-76-8 CAPLUS
CN 1,2-Benzenediol, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, monohydrobromide (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● xHBr

RN 157013-77-9 CAPLUS
CN 1,4-Benzenediol, 2-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, monohydrobromide (9CI) (CA INDEX NAMES)



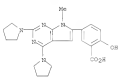
● HBr

RN 157013-78-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(2-fluoro-4-methoxyphenyl)-7-methyl-2,4-di-1-pyrrolidinyl-, monomethanesulfonate (9CI) (CA INDEX NAMES)

CM 1

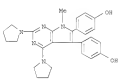
CRN 157012-67-4
CMF C22 H24 F N3 O

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HBr

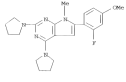
RN 157013-81-5 CAPLUS
CN Phenol, 4,4'-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidine-5,6-diyl)bis-, trihydrobromide (9CI) (CA INDEX NAMES)



● 3 HBr

RN 157013-82-6 CAPLUS
CN Phenol, 4-(7-methyl-2,4-di-1-piperazinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, trihydrobromide (9CI) (CA INDEX NAMES)

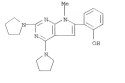
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 75-75-2
CMF C H4 O3 S

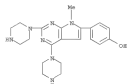
RN 157013-79-1 CAPLUS
CN Phenol, 2-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, monohydrobromide (9CI) (CA INDEX NAMES)



● HBr

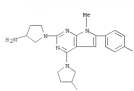
RN 157013-80-4 CAPLUS
CN Benzoic acid, 2-hydroxy-5-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, monohydrobromide (9CI) (CA INDEX NAMES)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● 3 HBr

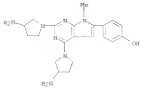
RN 157013-83-7 CAPLUS
CN 3-Pyrrolidinamine, 1,1'-[6-(4-methoxyphenyl)-7-methyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diyl]bis-, trihydrochloride (9CI) (CA INDEX NAMES)



● 3 HCl

RN 157013-84-8 CAPLUS
CN Phenol, 4-[2,4-bis(3-amino-1-pyrrolidinyl)-7-methyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl]-, trihydrobromide (9CI) (CA INDEX NAMES)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● HBr

RN 157013-85-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6,7-dimethyl-2,4-di-1-pyrrolidinyl-, monohydrochloride (9CI) (CA INDEX NAME)

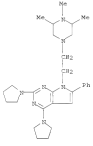
● AC1

RN 157013-86-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-ethyl-6-(1-methylethyl)-2,4-di-1-pyrrolidinyl-, sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 157013-33-9
CMF C19 H29 N5

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 110-16-7
CMF C4 H4 O4

Double bond geometry as shown.

RN 157013-88-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(3,5-dimethyl-1-piperazinyl)ethyl]-6-phenyl-2,4-di-1-pyrrolidinyl-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 157012-84-5
CMF C28 H39 N7

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 2

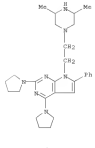
CRN 7664-93-9
CMF H2 O4 S

RN 157013-87-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-phenyl-2,4-di-1-pyrrolidinyl-7-[2-(3,4,5-trimethyl-1-piperazinyl)ethyl]-, (2E)-2-butenedioate (9CI) (CA INDEX NAME)

CM 1

CRN 157012-83-4
CMF C29 H41 N7

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



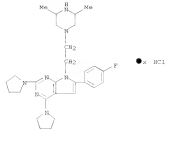
CM 2

CRN 110-16-7
CMF C4 H4 O4

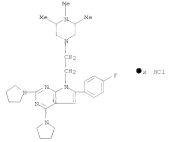
Double bond geometry as shown.

RN 157013-89-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(3,5-dimethyl-1-piperazinyl)ethyl]-6-(4-fluorophenyl)-2,4-di-1-pyrrolidinyl-, hydrochloride (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

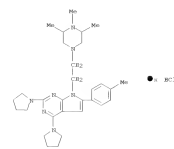


RN 157013-90-6 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 4-[4-(4-fluorophenyl)-2,4-di-1-pyrrolidinyl-7-[2-[3,4,5-trimethyl-1-piperazinyl]ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

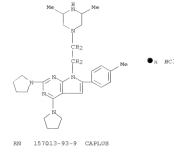


RN 157013-91-7 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 4-[4-methylphenyl]-2,4-di-1-pyrrolidinyl-7-[2-[3,4,5-trimethyl-1-piperazinyl]ethyl]-, hydrochloride (9CI) (CA INDEX

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
NAME)

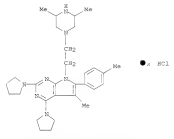


RN 157013-92-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-[3,5-dimethyl-1-piperazinyl]ethyl]-6-[4-methylphenyl]-2,4-di-1-pyrrolidinyl-, hydrochloride (9CI) (CA INDEX NAME)

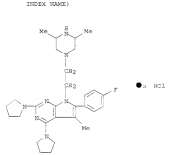


RN 157013-93-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-[3,5-dimethyl-1-piperazinyl]ethyl]-5-

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
methyl-6-(4-methylphenyl)-2,4-di-1-pyrrolidinyl-, hydrochloride (9CI) (CA INDEX NAME)

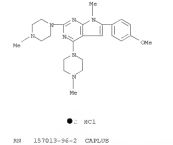


RN 157013-94-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-[2-(3,5-dimethyl-1-piperazinyl)ethyl]-6-(4-fluorophenyl)-5-methyl-2,4-di-1-pyrrolidinyl-, hydrochloride (9CI) (CA INDEX NAME)

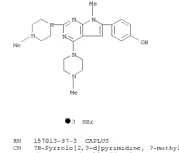


RN 157013-95-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-methoxyphenyl)-7-methyl-2,4-bis(4-methyl-1-piperazinyl)-, dihydrochloride (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

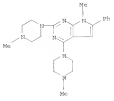


RN 157013-96-2 CAPLUS
CN Phenol, 4-[7-methyl-2,4-bis(4-methyl-1-piperazinyl)-7H-pyrrolo[2,3-d]pyrimidin-6-yl]-, trihydrobromide (9CI) (CA INDEX NAME)



RN 157013-97-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-methyl-2,4-bis(4-methyl-1-piperazinyl)-6-phenyl-, hydrochloride (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● x HCl

RN 157013-90-4 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-ethyl-6-methyl-2,4-di-1-pyrrolidinyl-, sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 157013-38-2
CMF C17 H25 N5

CM 2

CRN 7664-93-9
CMF H2 O4 S

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

● x HCl

RN 157014-92-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-(1,1-dimethylethyl)-6-(1-methylethyl)-2,4-di-1-pyrrolidinyl-, sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 157013-42-8
CMF C21 H33 N5

CM 2

CRN 7664-93-9
CMF H2 O4 S

RN 157014-03-4 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 6-(1-methylethyl)-2,4-di-1-pyrrolidinyl-, sulfate (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157013-99-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 7-ethyl-2,4-di-1-pyrrolidinyl-, sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 157013-39-3
CMF C16 H23 N5

CM 2

CRN 7664-93-9
CMF H2 O4 S

RN 157014-00-1 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 5,6,7-trimethyl-2,4-di-1-pyrrolidinyl-, hydrochloride (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CM 1

CRN 157013-43-9
CMF C17 H25 N5

CM 2

CRN 7664-93-9
CMF H2 O4 S

RN 157014-04-5 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-cyclopropyl-7-ethyl-2,4-di-1-pyrrolidinyl-, sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 157013-44-0
CMF C19 H27 N5

CM 2

CRN 7664-93-9

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 157014-03-6 CAPLUS
CN 1H-Pyrrolo[2,3-d]pyrimidine, 6-cyclopropyl-2,4-di-1-pyrrolidinyl-, sulfate (1:1) (9CI) (CA INDEX NAMES)

CM 1

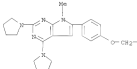
CRN 157017-45-3
CMF C17 H23 N5

CM 2

CRN 7664-93-9
CMF H2 O4 S

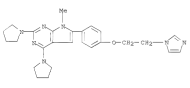
RN 157014-06-7 CAPLUS
CN Acetic acid, [4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)phenoxy]-, monohydrochloride (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● xCl

RN 157014-09-0 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-[4-[2-(1H-imidazol-1-yl)ethoxy]phenyl]-7-methyl-2,4-di-1-pyrrolidinyl-, hydrochloride (9CI) (CA INDEX NAME)



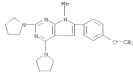
● x HCl

RN 157014-10-3 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-(4-bromophenyl)-7-methyl-2,4-di-1-pyrrolidinyl-, methanesulfonate (9CI) (CA INDEX NAME)

CM 1

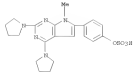
CRN 157013-12-2
CMF C21 H24 Br N5

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● xCl

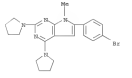
RN 157014-07-8 CAPLUS
CN Phenol, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, hydrogen sulfate (ester), potassium salt (9CI) (CA INDEX NAME)



● x

RN 157014-08-9 CAPLUS
CN Ethanamine, N,N-diethyl-2-[4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)phenoxy]-, monohydrochloride (9CI) (CA INDEX NAME)

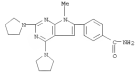
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

CRN 75-75-2
CMF C H4 O3 S

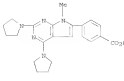
RN 157014-11-4 CAPLUS
CN Benzamide, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, hydrochloride (9CI) (CA INDEX NAME)



● x HCl

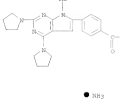
RN 157014-12-5 CAPLUS
CN Benzoic acid, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, potassium salt (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● H

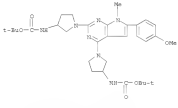
RN 157014-13-6 CAPLUS
CN Ethanesulfonic acid, 2-[[4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)benzoyl]amino]-, monoammonium salt (9CI) (CA INDEX NAME)



● NH_3

RN 157014-14-7 CAPLUS
CN Benzamide, 4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)-, dihydrochloride (9CI) (CA INDEX NAME)

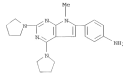
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157014-51-2 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-cyclopropyl-7-(phenylmethyl)-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

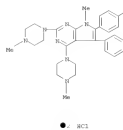
IT 157014-23-8P 157014-38-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for pyrrolopyrimidine drug)
RN 157014-23-8 CAPLUS
CN 1-Piperazinecarboxylic acid, 4,4'-[7-methyl-6-phenyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diyl]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



● 2 HCl

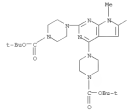
RN 157014-49-8 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 5,6-bis(4-methoxyphenyl)-7-methyl-2,4-bis[4-methyl-1-piperazinyl]-, dihydrochloride (9CI) (CA INDEX NAME)



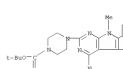
● 2 HCl

IT 157014-47-6P 157014-51-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as drug intermediate)
RN 157014-47-6 CAPLUS
CN Carbamic acid, [[6-(4-methoxyphenyl)-7-methyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diyl]bis[2,5-pyrrolidinediyl]]bis-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

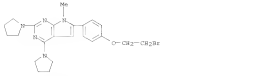


RN 157014-38-5 CAPLUS
CN 1-Piperazinecarboxylic acid, 4,4'-[5,6-bis(4-methoxyphenyl)-7-methyl-7H-pyrrolo[2,3-d]pyrimidine-2,4-diyl]bis-, bis(1,1-dimethylethyl) ester (9CI)
(CA INDEX NAME)

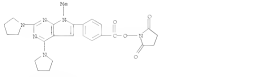


IT 157014-40-9P 157014-42-1P 157014-43-2P
157014-44-3P 157014-45-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, in preparation of pyrrolopyrimidine drug)
RN 157014-40-9 CAPLUS
CN 7H-Pyrrolo[2,3-d]pyrimidine, 6-[4-[2-bromoethoxy)phenyl]-7-methyl-2,4-di-1-pyrrolidinyl- (9CI) (CA INDEX NAME)

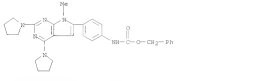
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157014-42-1 CAPLUS
CN 2,5-Pyrrolidinedione, 1-[[4-[7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl]benzoyl]oxy]- (9CI) (CA INDEX NAME)

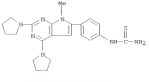


RN 157014-43-2 CAPLUS
CN Carbamic acid, [4-[7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl]phenyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

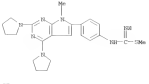


RN 157014-44-3 CAPLUS
CN Thiazoles, [4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)phenyl]- (9CI) (CA INDEX NAME)

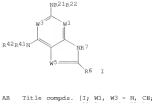
L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 157014-45-4 CAPLUS
CN Carbenimidothioic acid, [4-(7-methyl-2,4-di-1-pyrrolidinyl-7H-pyrrolo[2,3-d]pyrimidin-6-yl)phenyl]-, methyl ester (9CI) (CA INDEX NAME)



GI



AB Title compds. [I; W1, W2 = N, CR; W3 = N, CR3; R3, R6, R7 = H, (substituted) alkyl, cycloalkyl; R21, R22, R41, R42 = H, alkyl; R21R22N, R41R42N = (substituted) pyrrolidinyl, piperidinyl, morpholinyl, piperazinyl, aziridinyl, azetidinyl, imidazolyl, pyrazolyl, triazolyl, tetrazolyl, thiomorpholinyl, thiazolidinyl, etc.], were prepared for treating/preventing spinal trauma, head injury, subarachnoid hemorrhage, stroke, asthma, mucous formation/secretion, muscular dystrophy, adrianycin

L5 ANSWER 31 OF 31 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
cardiac toxicity, parkinsonism, Alzheimer's disease, multiple sclerosis, reperfusion damage, shock, burns, inflammatory disease, atherosclerosis, emphysema, lupus, cancer, ulcers, colitis, Crohn's disease, myocardial infarctions, ischemia, migraine, etc. (no data). I may be used similarly to glucocorticoids for treating the above conditions. Thus, 2,4,6-trichloropyrimidine was stirred with Me2NH2.HCl and (Me2CH)2NEt in THF to give 2,6-dichloro-4-methylaminopyrimidine. This was refluxed with pyrrolidine to give 4-methylamino-2,6-di-(1-pyrrolidinyl)pyrimidine. The latter was stirred with α-bromoacetophenone and (Me2CH)2NEt in MeCN to give 6-phenyl-2,4-di-(1-pyrrolidinyl)-7-methyl-7H-pyrrolo[2,3-d]pyrimidine.

=>

---Logging off of STN---

=>
Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	171.28	343.59

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-24.18	-24.18

STN INTERNATIONAL LOGOFF AT 16:36:21 ON 22 MAR 2007